Kernel Methods in Machine Learning

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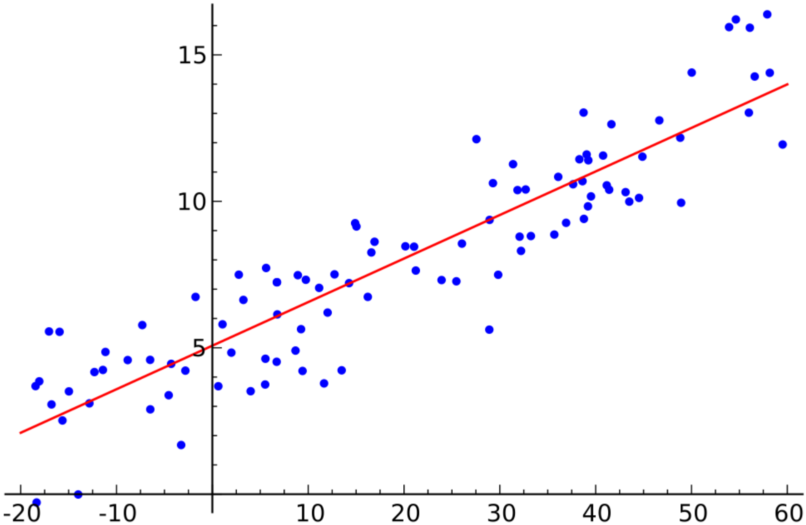
AMMI, May 2020

What we know how to solve



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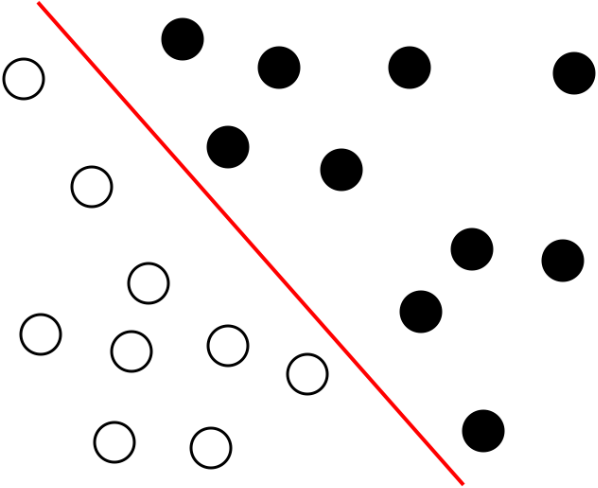
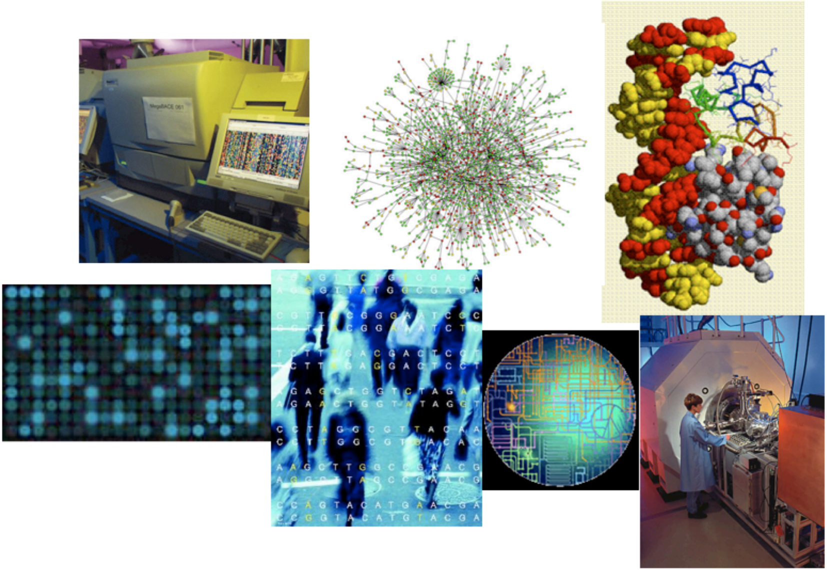
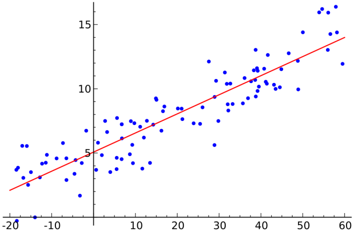
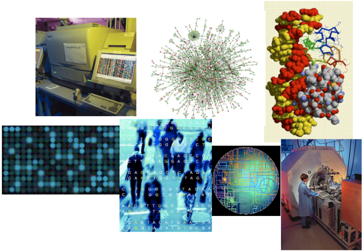


But real data are often more complicated...







Extend

well-understood, linear statistical learning techniques

to

real-world, complicated, structured, high-dimensional data

based on

a rigorous mathematical framework

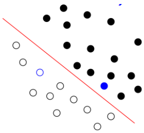
leading to

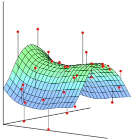
practical modelling tools and algorithms

Outline

Outline

General learning framework





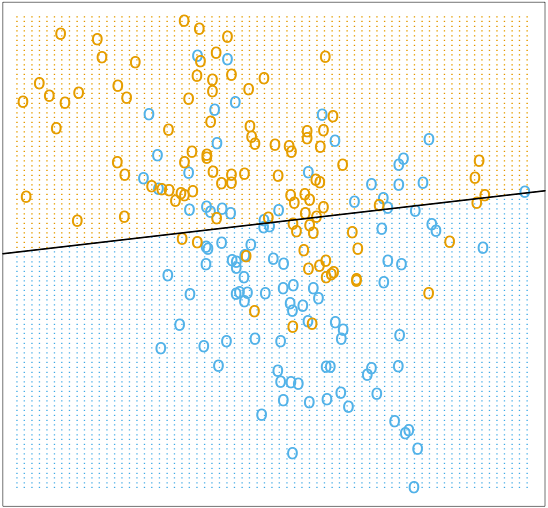
Input

- $\mathcal{X}$ the space of patterns or data (typically, $\mathcal{X} = \mathbb{R}^p$)
- $\mathcal{Y}$ the space of response or labels
  - Classification or pattern recognition : $\mathcal{Y} = \{-1, 1\}$
  - Regression : $\mathcal{Y} = \mathbb{R}$
  - Structured output: $\mathcal{Y}$ general
- $\mathcal{S} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ a training set in $(\mathcal{X} \times \mathcal{Y})^n$

Output

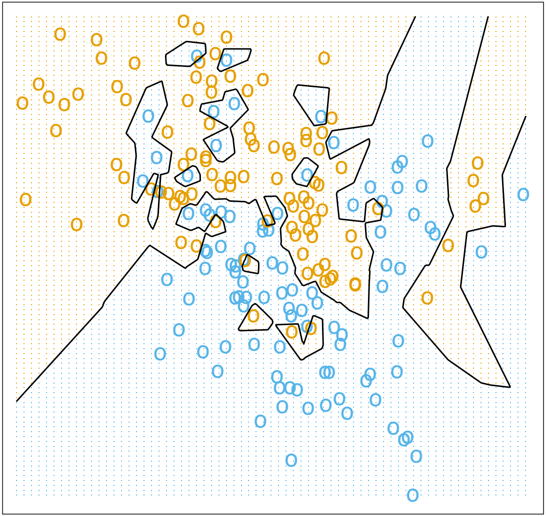
- A function $f : \mathcal{X} \to \mathcal{Y}$ to predict the output associated to any new pattern $x \in \mathcal{X}$ by $f(x)$

Simple example 1 : ordinary least squares (OLS)



(Hastie et al. The elements of statistical learning. Springer, 2001.)

Simple example 2 : 1-nearest neighbor (1-NN)



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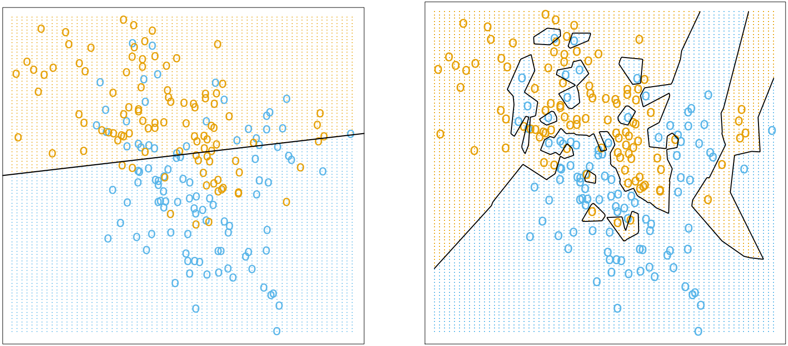
What's wrong?



- OLS: the linear separation is not appropriate = "large bias"
- 1-NN: the classifier seems too unstable = "large variance"

The fundamental "bias-variance" trade-off

- Assume $Y = f(X) + \epsilon$, where ϵ is some noise
- From the training set $\mathcal{S}$ we estimate the predictor $\hat{f}$
- On a new point x_0, we predict $\hat{f}(x_0)$ but the "true" observation will be $Y_0 = f(x_0) + \epsilon$
- On average, we make an error of:

$$
\begin{aligned}
& E_{\epsilon,\mathcal{S}} \left(Y_0 - \hat{f}(x_0) \right)^2 \\
& \quad = E_{\epsilon,\mathcal{S}} \left(f(x_0) + \epsilon - \hat{f}(x_0) \right)^2 \\
& \quad = E\epsilon^2 + E_{\mathcal{S}} \left(f(x_0) - \hat{f}(x_0) \right)^2 \\
& \quad = E\epsilon^2 + \left(f(x_0) - E_{\mathcal{S}}\hat{f}(x_0) \right)^2 + E_{\mathcal{S}} \left(\hat{f}(x_0) - E_{\mathcal{S}}\hat{f}(x_0) \right)^2 \\
& \quad = \mathit{noise} + \mathit{bias}^2 + \mathit{variance}
\end{aligned}
$$

Important message

Future prediction error = noise + bias^2 + variance

- The "noise" part can not be avoided
- By choosing a learning model, we should consider both "bias" and "variance" if we want to make good predictions
- Intuitively, a more realistic, more complex model with more parameters to estimate has smaller bias but larger variance
- If variance dominates bias (eg, in high dimension), then having more complex, more realist models can hurt performance
- In other words, a wrong but simple model can work better than a more realistic but more complex model
- In many applications, domain experts (non-statisticians) often ignore the cost of complexity and prefer complex models, which can lead to disappointing results. You can help them!

Back to OLS

- Linear model with parameter $\beta \in \mathbb{R}^p$:

$$\forall x \in \mathbb{R}^p , \quad f_\beta(x) = \beta^\top x \quad \left(= \sum_{i=1}^{p} \beta_i x_i \right)$$

- Estimate $\hat{\beta}^{OLS}$ from training data to minimize the mean sum of squares (MSE):

$$\mathrm{MSE}(\beta) = \frac{1}{n} \sum_{i=1}^{n} (y_i - f_\beta(x_i))^2$$

Back to OLS (cont.)

- Let's use matrix notations:
  - $Y = (y_1, \ldots, y_n)^\top \in \mathbb{R}^n$ the vector of outcomes
  - $X = (x_1, \ldots, x_n)^\top \in \mathbb{R}^{n \times p}$ the matrix (n rows=samples, p columns=features)
- We can rewrite MSE as

$$\mathrm{MSE}(\beta) = \frac{1}{n} (Y - X\beta)^\top (Y - X\beta)$$

- $\mathrm{MSE}(\beta)$ is a quadratic convex function; we minimize it by setting its gradient to 0:

$$\nabla_\beta \mathrm{MSE}(\beta) = \frac{2}{n} X^\top (X\beta - Y) = 0$$

- If $X^\top X$ is non-singular, the minimum is reached at

$$\hat{\beta}^{OLS} = \operatorname*{argmin}_\beta \mathrm{MSE}(\beta) = \left(X^\top X\right)^{-1} X^\top Y$$

Properties of OLS

Bias and variance of OLS

- Assume $Y = X\beta^* + \epsilon$, where $E\epsilon = 0$ and $E\epsilon\epsilon^\top = \sigma^2 I$.
- Then the least squares estimator

$$\hat{\beta}^{OLS} = \left(X^\top X\right)^{-1} X^\top Y$$

satisfies

$$\begin{cases} E\left(\hat{\beta}^{OLS}\right) = \beta^*, \\ Var(\hat{\beta}^{OLS}) = E\left(\hat{\beta}^{OLS} - \beta^*\right)\left(\hat{\beta}^{OLS} - \beta^*\right)^\top = \sigma^2 \left(X^\top X\right)^{-1}. \end{cases}$$

Proof: exercice

Optimality of OLS

Gauss-Markov theorem

- Assume $Y = X\beta^* + \epsilon$, where $E\epsilon = 0$ and $E\epsilon\epsilon^\top = \sigma^2 I$.
- Then the least squares estimator $\hat{\beta}^{OLS}$ is BLUE (best linear unbiased estimator), i.e., for any other estimator $\tilde{\beta} = CY$ with $E\tilde{\beta} = \beta^*$,

$$Var(\hat{\beta}^{OLS}) \preccurlyeq Var(\tilde{\beta}) \quad \left(\Leftrightarrow \forall x_0\,,\, Var(x_0^\top \hat{\beta}^{OLS}) \leq Var(x_0^\top \tilde{\beta})\right)$$

Proof: exercice

- For $\tilde{\beta} = CY$, define $D = C - \left(X^\top X\right)^{-1} X^\top$
- Show that if $\tilde{\beta}$ is unbiased, then $DX = 0$
- Show that $Var(\tilde{\beta}) = Var(\hat{\beta}^{OLS}) + \sigma^2 DD^\top$

Is BLUE good enough?

OLS mean prediction variance

Suppose $(x_i, y_i)_{i=0,\dots,n}$ are i.i.d. random pairs that follow a distribution (x, y) with

$$Ex = 0\,, \quad Exx^\top = C\,,$$
$$y = x^\top \beta^* + \epsilon\,, \quad E\epsilon = 0\,, \quad E\epsilon^2 = 1\,,$$

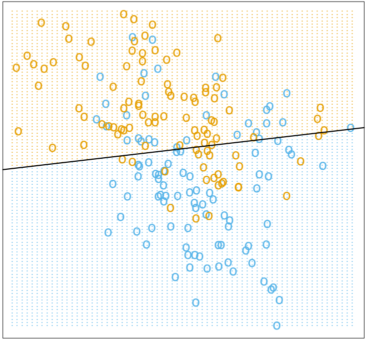
then

$$E_{\mathcal{S},x_0} Var(f(x_0)) = E_{\mathcal{S},x_0} Var(x_0^\top \hat{\beta}^{OLS}) = \frac{\sigma^2 p}{n}\,.$$

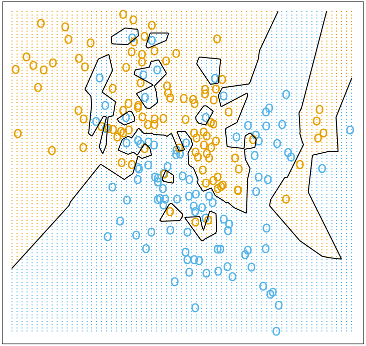
Proof:

$$\begin{aligned}
E_{\mathcal{S},x_0} Var(x_0^\top \hat{\beta}^{OLS}) &= \sigma^2 E_{\mathcal{S},x_0}\left[x_0^\top (X^\top X)^{-1} x_0\right] \\
&= \sigma^2 E_{\mathcal{S},x_0} \text{Trace}\left[(X^\top X)^{-1} x_0 x_0^\top\right] \\
&= \sigma^2 \text{Trace}\left[E_{\mathcal{S}}(X^\top X)^{-1} \times E_{x_0} x_0 x_0^\top\right] \\
&= \sigma^2 \text{Trace}\left[(nC)^{-1} \times C\right] \\
&= \sigma^2 p/n
\end{aligned}$$

The curse of dimensionality



Small dimension



Large dimension

- In high dimensions, variance dominates, even for simple linear estimators.
- BLUE estimators are therefore useless.
- In that case, we may have smaller total risk by increasing bias and decreasing variance

A solution: shrinkage estimators

1. Define a large family of "candidate classifiers", e.g., linear predictors:

$$f_\beta(x) = \beta^\top x \quad \text{for } x \in \mathbb{R}^p$$

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2. For any candidate classifier f_β, quantify how "good" it is on the training set with some empirical risk, e.g.:

$$R(\beta) = \frac{1}{n}\sum_{i=1}^{n}(f_\beta(x_i) - y_i)^2 \, .$$

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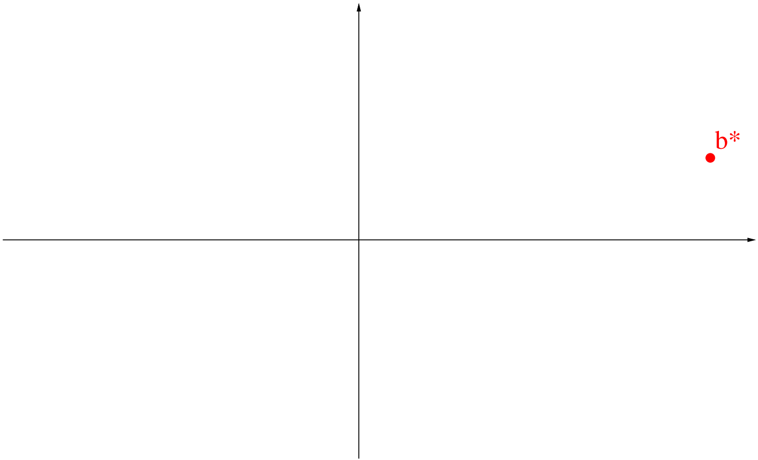
3. Choose β that achieves the minimum empirical risk, subject to some constraint:

$$\min_\beta R(\beta) \quad \text{subject to} \quad \Omega(\beta) \leq C \, ,$$

for some penalty function $\Omega : \mathbb{R}^p \to \mathbb{R}^+$ and $C \geq 0$.

Why skrinkage classifiers?

$$\min_{\beta} R(\beta) \quad \text{subject to} \quad \Omega(\beta) \leq C\,.$$



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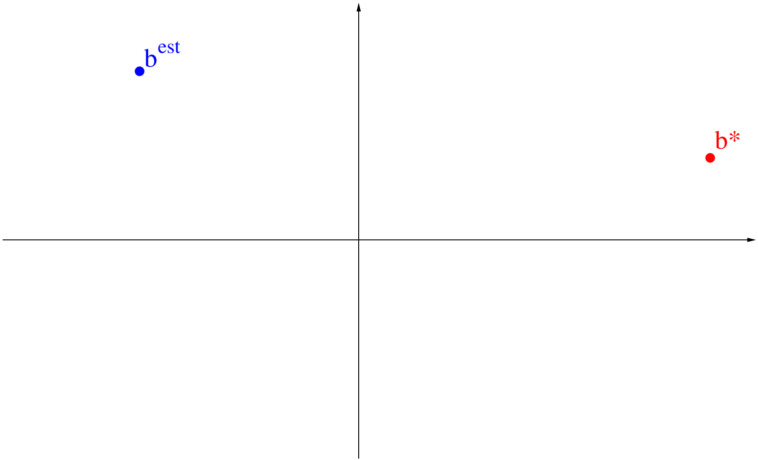

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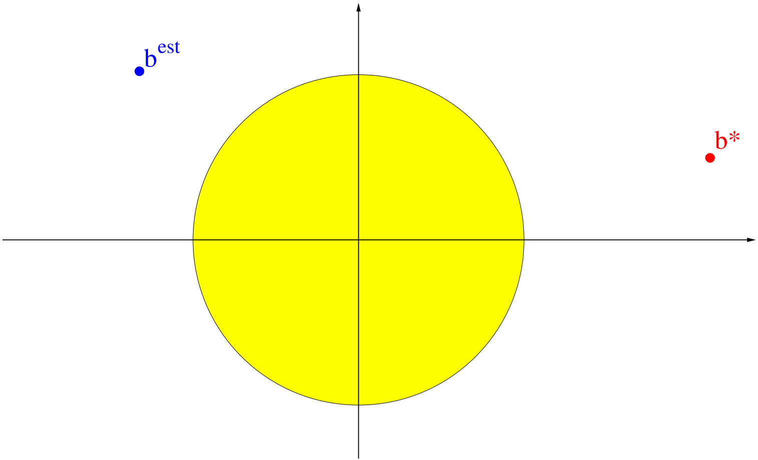

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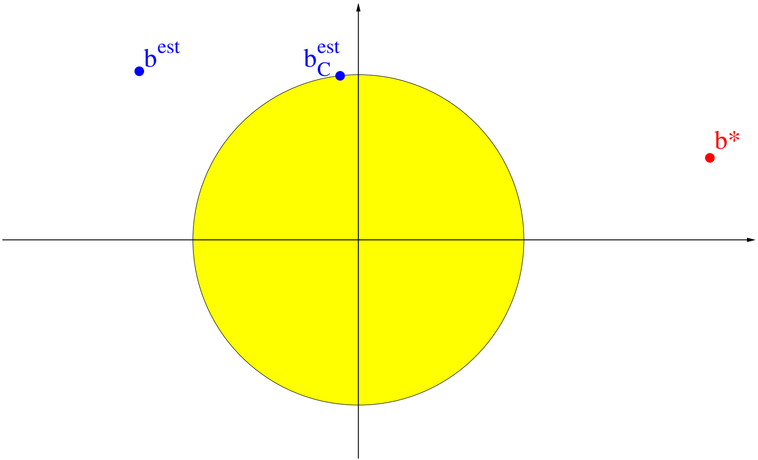

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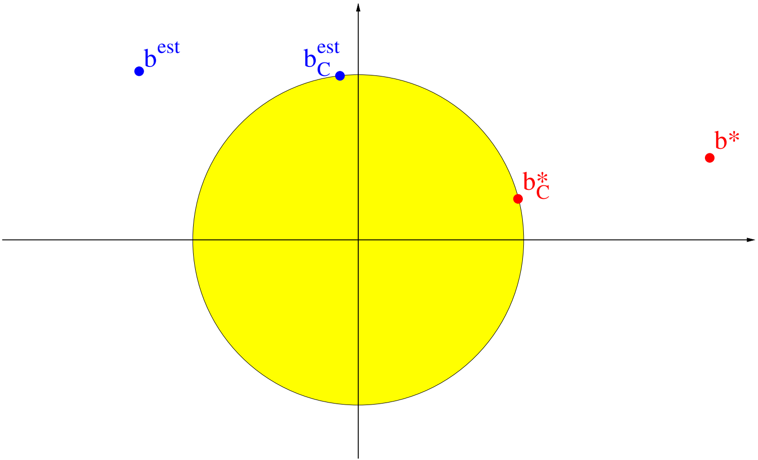

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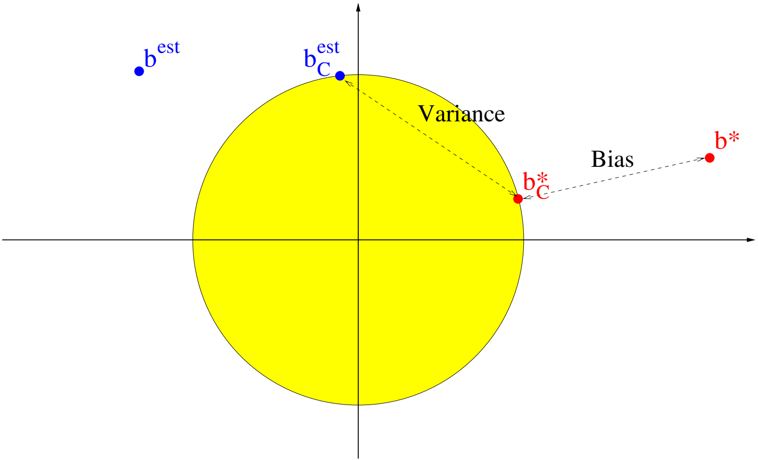

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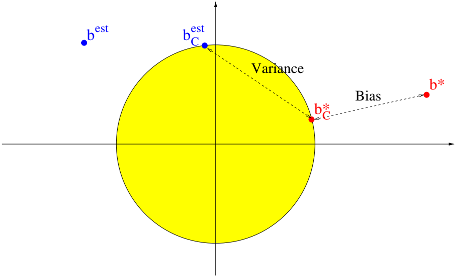

"Increases bias and decreases variance"

Choice of Ω can decrease the bias

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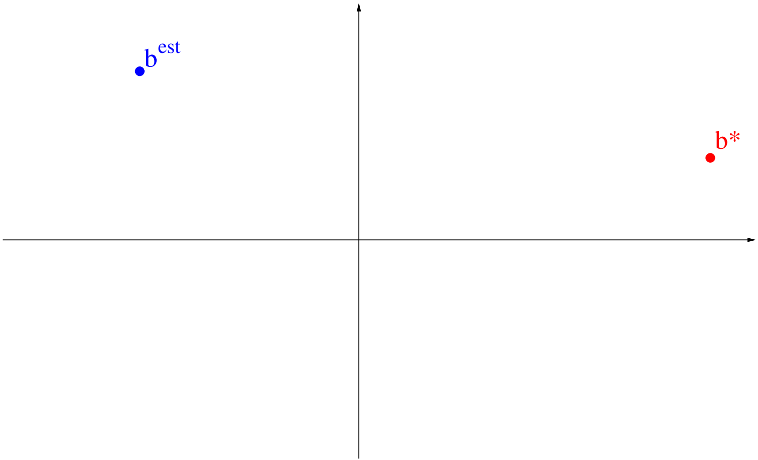

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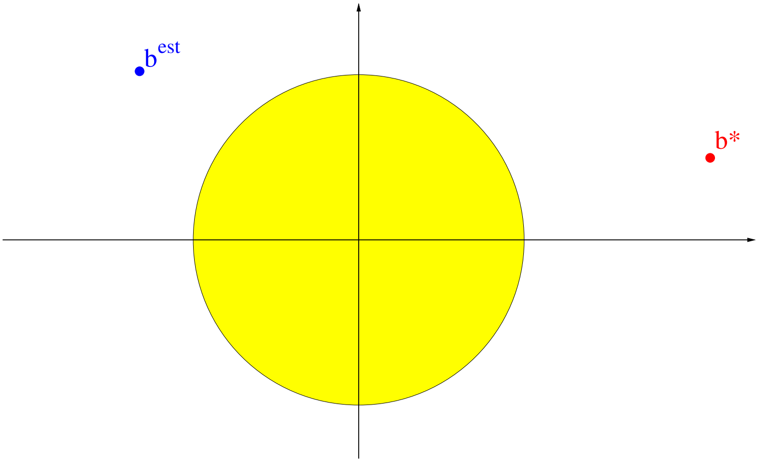

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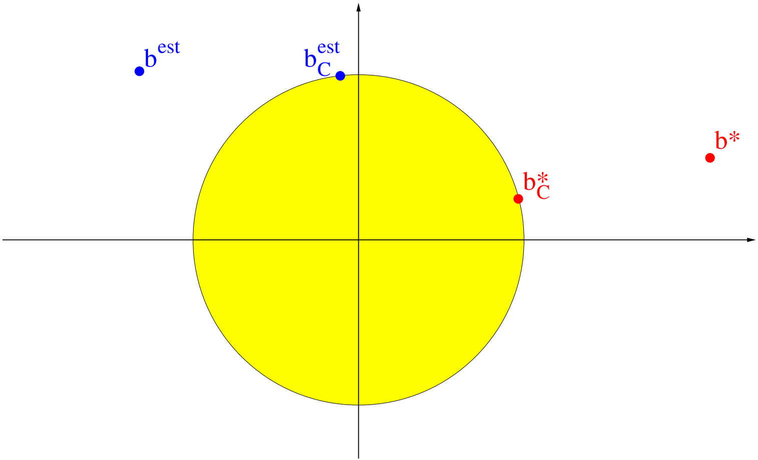

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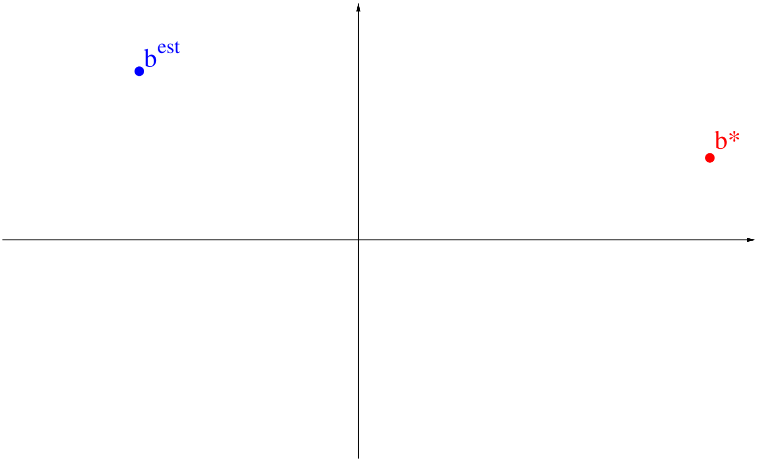

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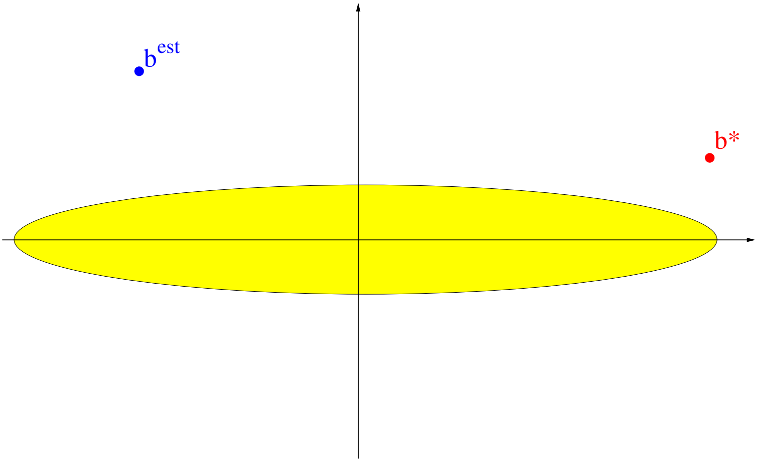

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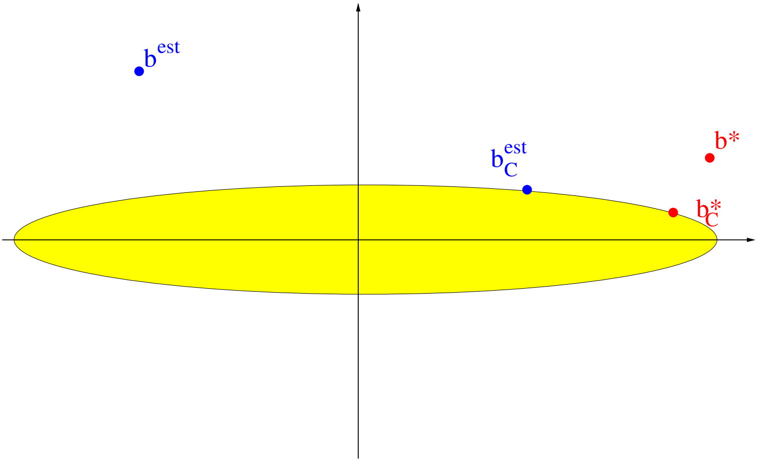


Equivalent formulation

$$\min_{\beta} R(\beta) \quad \text{subject to} \quad \Omega(\beta) \leq C$$

is equivalent to

$$\min_{\beta} R(\beta) + \lambda\Omega(\beta)$$

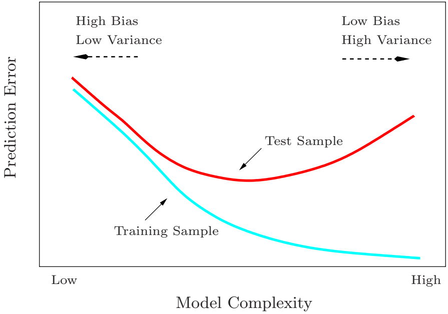
- There exists a (not necessarily unique) correspondance between C and λ such that the solutions to both problems are the same.
- If C increase, λ decreases
- The formulation with λ is often preferred to implement the algorithm
- Proof: using Lagrangian duality (only true under some assumptions, eg, R and Ω convex + Slater conditions, see later)

Choice of C or λ

- Choose a grid of values Λ for λ (or C)
- For each $\lambda \in \Lambda$ (or C) estimate the best model

$$\hat{\beta}_\lambda \in \underset{\beta}{\operatorname{argmin}}\ R(\beta) + \lambda\Omega(\beta)$$

- Select $\hat{\beta} = \hat{\beta}_{\hat{\lambda}}$ to minimize the bias-variance tradeoff.



Cross-validation

A simple and systematic procedure to estimate the risk (and to optimize the model's parameters)

1. Randomly divide the training set (of size n) into K (almost) equal portions, each of size K/n
2. For each portion, fit the model with different parameters on the $K-1$ other groups and test its performance on the left-out group
3. Average performance over the K groups, and take the parameter with the smallest average performance.

Taking $K = 5$ or 10 is recommended as a good default choice.

Summary

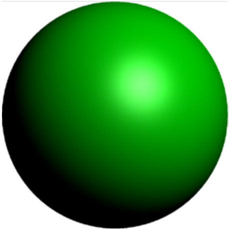
1. Many problems in modern machine learning involve models with many parameters (i.e., high dimension)
2. The total prediction error of a learning system is the sum of a bias and a variance error
3. In high dimension, the variance term often dominates
4. Shrinkage methods allow us to control the bias/variance trade-off
5. The choice of the penalty is where we can put prior knowledge to decrease bias
6. The parameter to control the bias-variance trade-off (C or λ) is typically chosen by cross-validation, to minimize the test error.

Outline

Overview

- We focus on a simple penalty function: the squared Euclidean norm

$$\Omega(\beta) = \| \beta \|^2 \quad \left(= \beta^\top \beta = \sum_{i=1}^{p} \beta_i^2 \right)$$



- This will allow us to derive many state-of-the-art linear methods:
  - Ridge regression
  - Ridge logistic regression
  - SVM and large-margin classifiers
- This will allow us to extend these linear methods to nonlinear models, using kernels

Outline

Ridge regression (Hoerl and Kennard, 1970)

1. Consider the set of linear predictors:

$$\forall \beta \in \mathbb{R}^p, \quad f_\beta(x) = \beta^\top x \quad \text{for } x \in \mathbb{R}^p.$$

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2. Consider the MSE as empirical risk:

$$R(\beta) = \frac{1}{n} \sum_{i=1}^{n} (f_\beta(x_i) - y_i)^2 .$$

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2. Consider the MSE as empirical risk:

$$R(\beta) = \frac{1}{n}\sum_{i=1}^{n}(f_\beta(x_i) - y_i)^2\,.$$

3. Consider the squared Euclidean norm as a penalty:

$$\Omega(\beta) = \|\,\beta\,\|^2\,.$$

Solution

- The penalized risk can be written in matrix form:

$$
\begin{aligned}
R(\beta) + \lambda\Omega(\beta) &= \frac{1}{n}\sum_{i=1}^{n}\left(f_\beta\left(x_i\right) - x_i\right)^2 + \lambda\sum_{i=1}^{p}\beta_i^2 \\
&= \frac{1}{n}\left(Y - X\beta\right)^\top\left(Y - X\beta\right) + \lambda\beta^\top\beta\,.
\end{aligned}
$$

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- Unique minimizer (by setting the gradient to 0):

$$\hat{\beta}_\lambda^{\text{ridge}} = \arg\min_{\beta\in\mathbb{R}^p}\left\{R(\beta) + \lambda\Omega(\beta)\right\} = \left(X^\top X + \lambda n I\right)^{-1} X^\top Y\,.$$

Performance of ridge regression

Lemma

Assume that:

- $Y = X\beta^* + \epsilon$, where $E\epsilon = 0$ and $E\epsilon\epsilon^\top = \sigma^2 I$.
- $X^\top X = nI_p$ (orthogonal design)

Then:

$$\begin{cases} bias\left(\hat{\beta}_\lambda^{\text{ridge}}\right) = E\left(\hat{\beta}_\lambda^{\text{ridge}}\right) - \beta^* = -\frac{\lambda}{1+\lambda}\beta^*\,, \\ Var(\hat{\beta}_\lambda^{\text{ridge}}) = \frac{\sigma^2}{n(1+\lambda)^2} I_p = \frac{1}{(1+\lambda)^2} Var(\hat{\beta}^{OLS})\,. \end{cases}$$

Proof: exercice

Performance of ridge regression

Corollary

For any $\lambda \geq 0$ let

$$f(\lambda) = E_{\mathcal{S},x_0}\left[bias^2\left(x_0^\top \hat{\beta}_\lambda^{\text{ridge}}\right) + Var\left(x_0^\top \hat{\beta}_\lambda^{\text{ridge}}\right)\right]$$

where $Ex_0 = 0, Ex_0x_0^\top = I_p$. Then $f(\lambda)$ is minimum for

$$\lambda^* = \frac{\sigma^2 p}{n\|\beta^*\|^2}$$

and

$$f(\lambda^*) = \frac{f(0)f(+\infty)}{f(0)+f(+\infty)} \leq \min\left\{f(0), f(\infty)\right\}$$

where

$$f(0) = \sigma^2 p/n\,, \quad f(\infty) = \|\beta^*\|^2$$

Proof: exercice

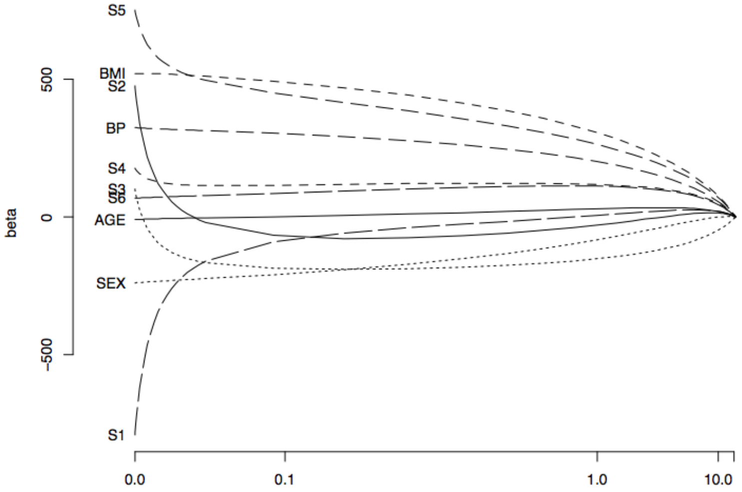
Limit cases

$$\hat{\beta}_{\lambda}^{\text{ridge}} = \left(X^{\top}X + \lambda n I\right)^{-1} X^{\top} Y$$

Corollary

- As $\lambda \to 0$, $\hat{\beta}_{\lambda}^{\text{ridge}} \to \hat{\beta}^{\text{OLS}}$ (low bias, high variance).
- As $\lambda \to +\infty$, $\hat{\beta}_{\lambda}^{\text{ridge}} \to 0$ (high bias, low variance).

Ridge regression example



(From Hastie et al., 2001)

Ridge regression with correlated features

Ridge regression is particularly useful in the presence of correlated features:

```
> library(MASS) # for the lm.ridge command
> x1 <- rnorm(20)
> x2 <- rnorm(20,mean=x1,sd=.01)
> y <- rnorm(20,mean=3+x1+x2)
> lm(y~x1+x2)$coef
(Intercept)          x1          x2
   3.070699   25.797872  -23.748019
> lm.ridge(y~x1+x2,lambda=1)
                 x1        x2
3.066027 1.015862 0.956560
```

Generalization: ℓ_2-regularized learning

- A general ℓ_2-penalized estimator is of the form

$$\min_{\beta} \left\{ R(\beta) + \lambda \| \beta \|^2 \right\} , \tag{1}$$

  where

$$R(\beta) = \frac{1}{n} \sum_{i=1}^{n} \ell(f_\beta(x_i), y_i)$$

  for some general loss functions ℓ.

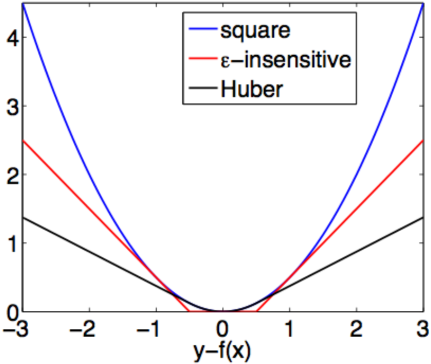
- Ridge regression corresponds to the particular loss

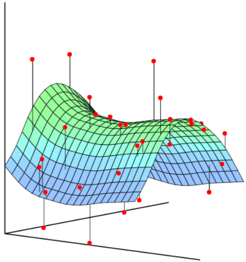
$$\ell(u, y) = (u - y)^2 .$$

- For general, convex losses, the problem (1) is strictly convex and has a unique global minimum, which can usually be found by numerical algorithms for convex optimization.

Losses for regression

- Square loss : $\ell(u, y) = (u - y)^2$
- ϵ-insensitive loss : $\ell(u, y) = (|\, u - y\,| - \epsilon)_+$
- Huber loss : mixed quadratic/linear



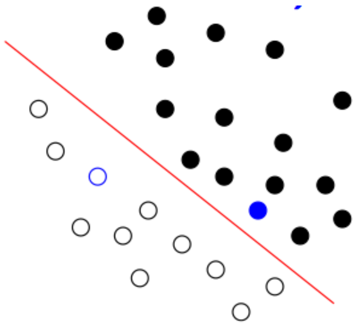


Outline

Binary classification

Setting

- $\mathcal{X} = \mathbb{R}^p$ set of inputs
- $\mathcal{Y} = \{-1, 1\}$ binary outputs
- $\mathcal{S} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ a training set in $(\mathcal{X} \times \mathcal{Y})^n$
- Goal: Estimate a function $f : \mathcal{X} \to \mathbb{R}$ to predict y by $\mathit{sign}(f(x))$



The 0/1 loss

- The 0/1 loss measures if a prediction is correct or not:

$$\ell_{0/1}(f(x), y)) = \mathbf{1}(yf(x) < 0) = \begin{cases} 0 & \text{if } y = sign(f(x)) \\ 1 & \text{otherwise.} \end{cases}$$

- It is them tempting to learn $f_\beta(x) = \beta^\top x$ by solving:

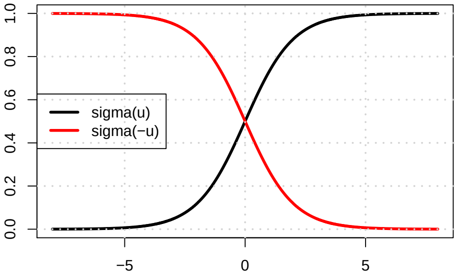
$$\min_{\beta \in \mathbb{R}^p} \underbrace{\frac{1}{n} \sum_{i=1}^{n} \ell_{0/1}(f_\beta(x_i), y_i)}_{\text{misclassification rate}} + \underbrace{\lambda \| \beta \|^2}_{\text{regularization}}$$

- However:
  - The problem is non-smooth, and typically NP-hard to solve
  - The regularization has no effect since the 0/1 loss is invariant by scaling of β
  - In fact, no function achieves the minimum when $\lambda > 0$ (*why?*)

The logistic loss

- An alternative is to define a probabilistic model of y parametrized by $f(x)$, e.g.:

$$\forall y \in \{-1,1\}, \quad p(y \mid f(x)) = \frac{1}{1+e^{-yf(x)}} = \sigma(yf(x))$$



- The logistic loss is the negative conditional likelihood:

$$\ell_{logistic}(f(x), y) = -\ln p(y \mid f(x)) = \ln\left(1+e^{-yf(x)}\right)$$

Ridge logistic regression (Le Cessie and van Houwelingen, 1992)

$$\min_{\beta \in \mathbb{R}^p} J(\beta) = \frac{1}{n} \sum_{i=1}^{n} \ln\left(1 + e^{-y_i \beta^\top x_i}\right) + \lambda \|\beta\|^2$$

- Can be interpreted as a regularized conditional maximum likelihood estimator
- No explicit solution, but smooth convex optimization problem that can be solved numerically

Solving ridge logistic regression

$$\min_{\beta} J(\beta) = \frac{1}{n}\sum_{i=1}^{n} \ln\left(1 + e^{-y_i \beta^\top x_i}\right) + \lambda \|\beta\|^2$$

No explicit solution, but convex problem with:

$$\begin{aligned}
\nabla_\beta J(\beta) &= -\frac{1}{n}\sum_{i=1}^{n} \frac{y_i x_i}{1 + e^{y_i \beta^\top x_i}} + 2\lambda\beta \\
&= -\frac{1}{n}\sum_{i=1}^{n} y_i \left[1 - P_\beta(y_i \mid x_i)\right] x_i + 2\lambda\beta \\
\nabla_\beta^2 J(\beta) &= \frac{1}{n}\sum_{i=1}^{n} \frac{x_i x_i^\top e^{y_i \beta^\top x_i}}{\left(1 + e^{y_i \beta^\top x_i}\right)^2} + 2\lambda I \\
&= \frac{1}{n}\sum_{i=1}^{n} P_\beta(1 \mid x_i)\left(1 - P_\beta(1 \mid x_i)\right) x_i x_i^\top + 2\lambda I
\end{aligned}$$

Solving ridge logistic regression (cont.)

$$\min_{\beta} J(\beta) = \frac{1}{n} \sum_{i=1}^{n} \ln\left(1 + e^{-y_i \beta^\top x_i}\right) + \lambda \|\beta\|^2$$

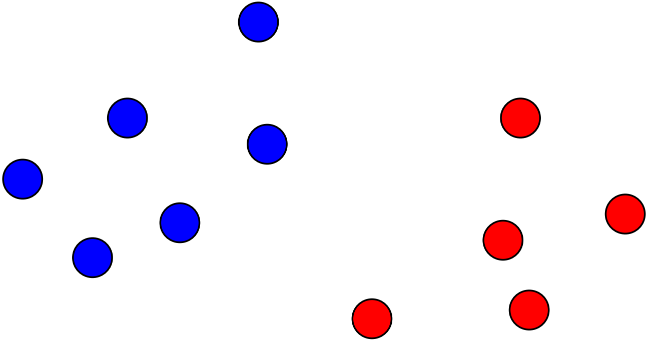
- The solution can then be found by Newton-Raphson iterations:

$$\beta^{new} \leftarrow \beta^{old} - \left[\nabla_\beta^2 J\left(\beta^{old}\right)\right]^{-1} \nabla_\beta J\left(\beta^{old}\right).$$

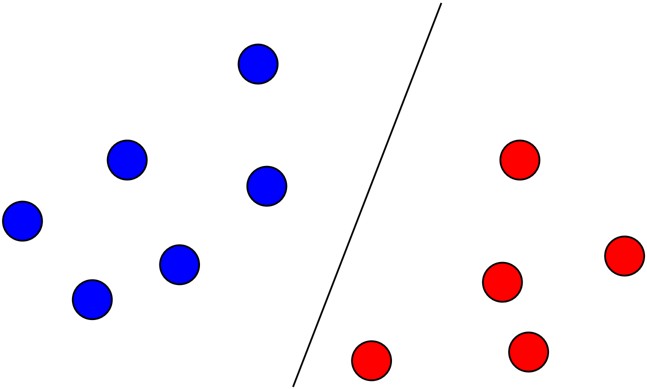
- Each step is equivalent to solving a weighted ridge regression problem (*left as exercise*)
- This method is therefore called iteratively reweighted least squares (IRLS).

Outline

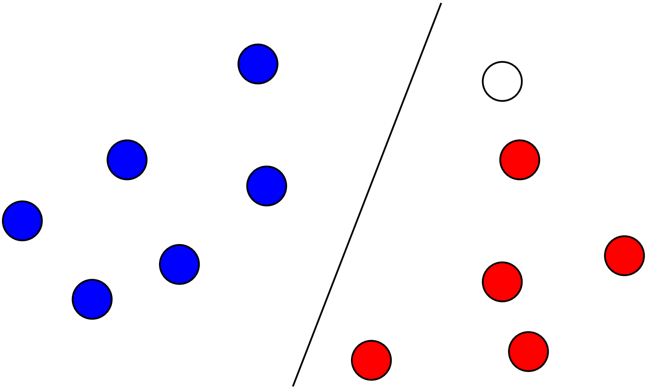
Linear classifier



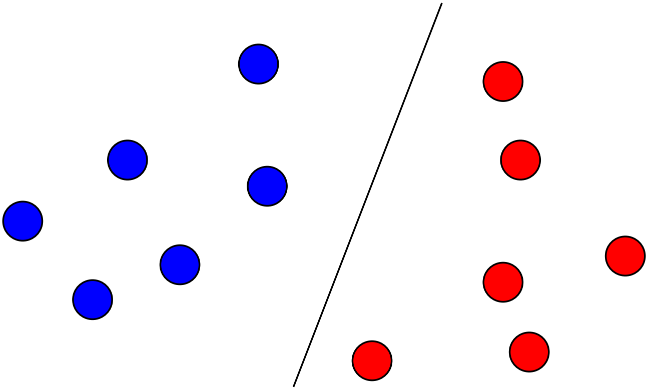
Linear classifier



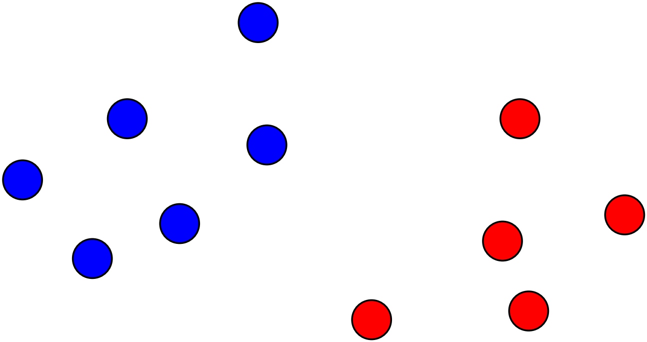
Linear classifier



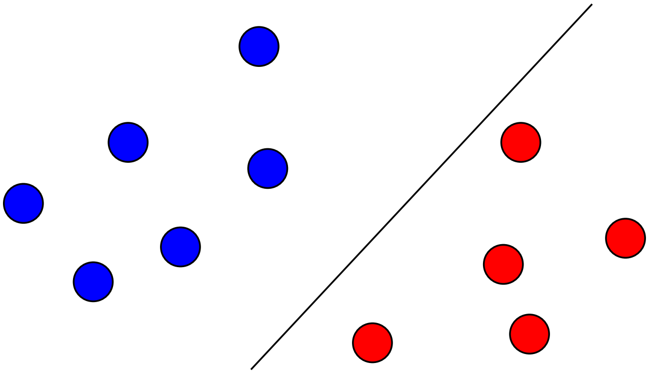
Linear classifier



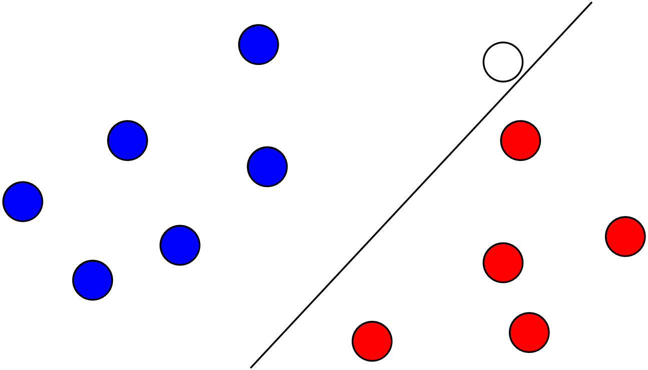
Linear classifier



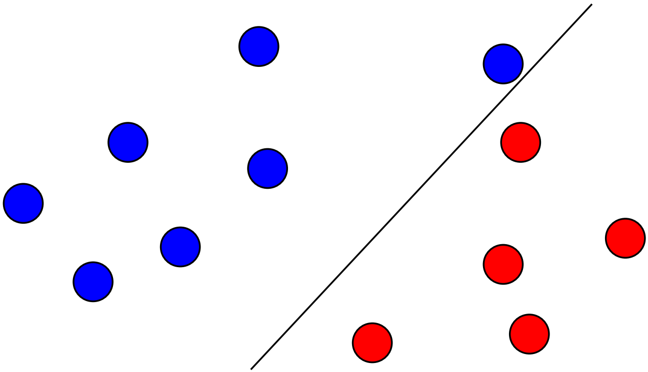
Linear classifier



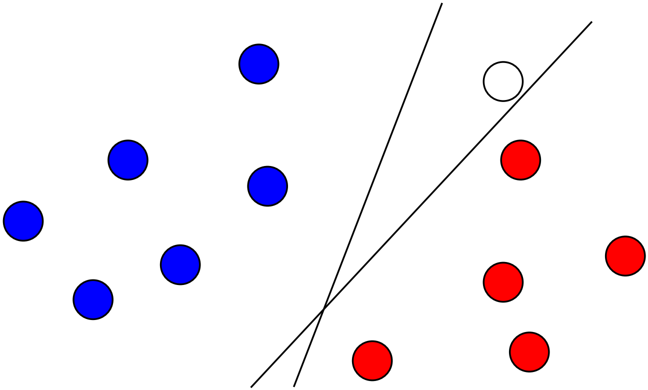
Linear classifier



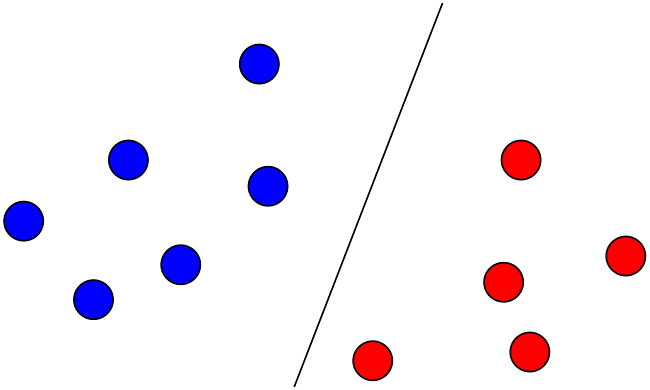
Linear classifier



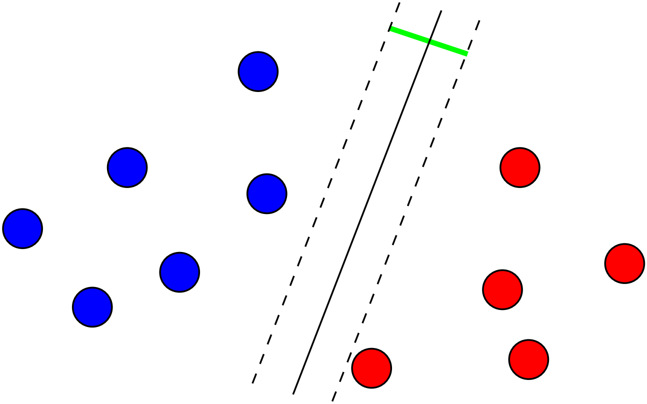
Which one is better?



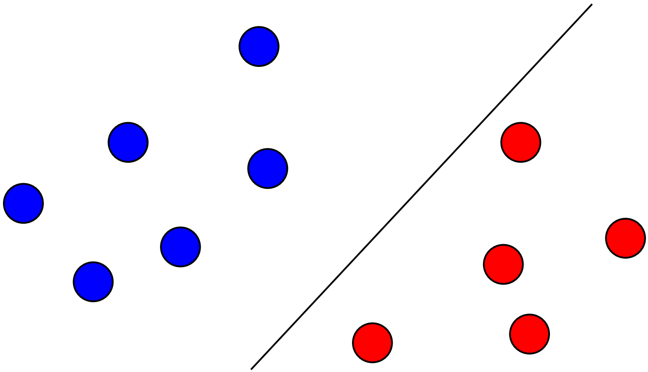
The margin of a linear classifier



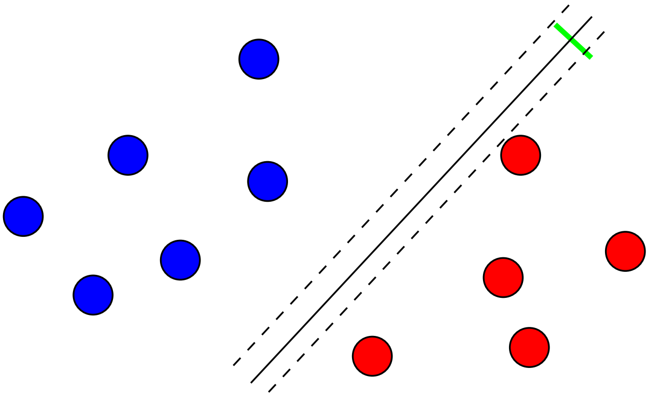
The margin of a linear classifier

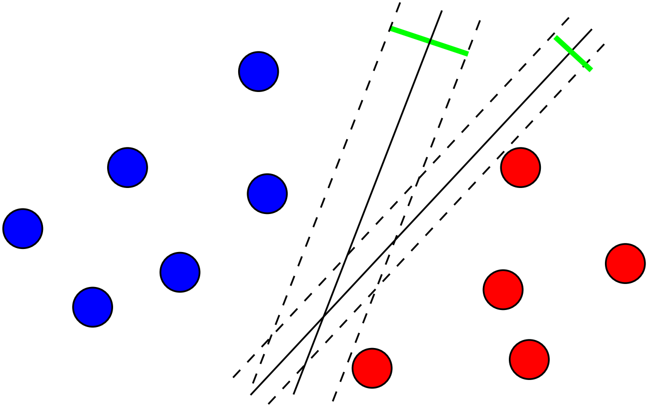


The margin of a linear classifier

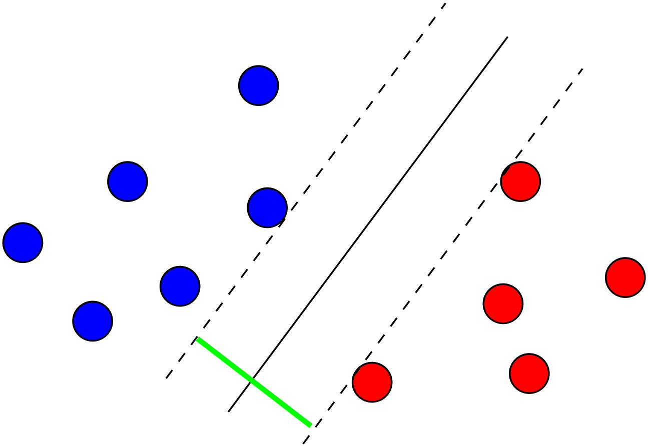


The margin of a linear classifier

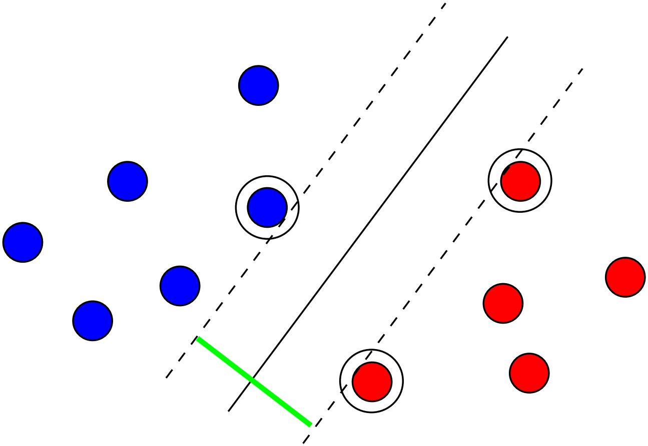




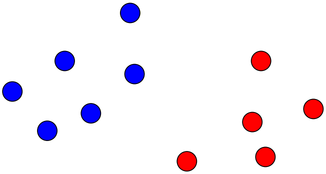
Largest margin classifier (*hard-margin SVM*)



Support vectors



More formally



- The training set is a finite set of n data/class pairs:

$$\mathcal{S} = \{(x_1, y_1), \ldots, (x_n, y_n)\} \ ,$$

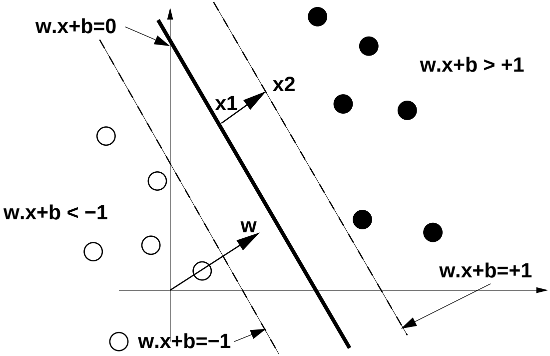
where $x_i \in \mathbb{R}^p$ and $y_i \in \{-1, 1\}$.

- We assume (for the moment) that the data are linearly separable, i.e., that there exists $(w, b) \in \mathbb{R}^p \times \mathbb{R}$ such that:

$$\begin{cases} w^\top x_i + b > 0 & \text{if } y_i = 1\,, \\ w^\top x_i + b < 0 & \text{if } y_i = -1\,. \end{cases}$$

How to find the largest separating hyperplane?

For a given linear classifier $f(x) = w^\top x + b$ consider the "tube" defined by the values -1 and $+1$ of the decision function:



The margin is $2/\| w \|$

Indeed, the points x_1 and x_2 satisfy:

$$\begin{cases} w^\top x_1 + b = 0\,, \\ w^\top x_2 + b = 1\,. \end{cases}$$

By subtracting we get

$$w^\top (x_2 - x_1) = 1 = \| w \| \times \| x_2 - x_1 \|\,,$$

and therefore:

$$\gamma = 2\| x_2 - x_1 \|_2 = \frac{2}{\| w \|}\,.$$

All training points should be on the correct side of the dotted line

For positive examples ($y_i = 1$) this means:

$$w^\top x_i + b \geq 1\,.$$

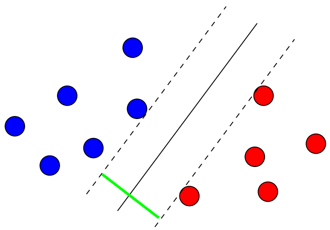
For negative examples ($y_i = -1$) this means:

$$w^\top x_i + b \leq -1\,.$$

Both cases are summarized by:

$$\forall i = 1, \ldots, n\,, \qquad y_i \left(w^\top x_i + b \right) \geq 1\,.$$

Finding the optimal hyperplane



Find (w, b) which minimize:

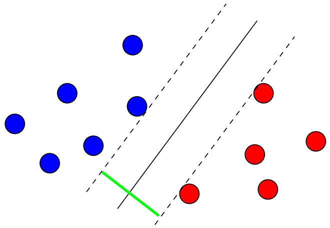
$$\| w \|^2$$

under the constraints:

$$\forall i = 1, \ldots, n, \qquad y_i \left(w^\top x_i + b \right) - 1 \geq 0 \,.$$

This is a classical quadratic program on $\mathbb{R}^{p+1}$.

Another view of hard-margin SVM



$$\min_{w,b} \left\{ \sum_{i=1}^{n} \ell_{hard-margin}\left(w^\top x_i + b, y_i\right) + \lambda \| w \|^2 \right\},$$

for the hard-margin loss function:

$$\ell_{hard-margin}(u, y) = \begin{cases} 0 & \text{if } yu \geq 1, \\ +\infty & \text{otherwise.} \end{cases}$$

Outline

Optimization problems

Setting

- We consider an equality and inequality constrained optimization problem over a variable $x \in \mathcal{X}$:

$$\begin{aligned} \text{minimize} \quad & f(x) \\ \text{subject to} \quad & h_i(x) = 0 \,, \quad i = 1, \ldots, m \,, \\ & g_j(x) \leq 0 \,, \quad j = 1, \ldots, r \,, \end{aligned}$$

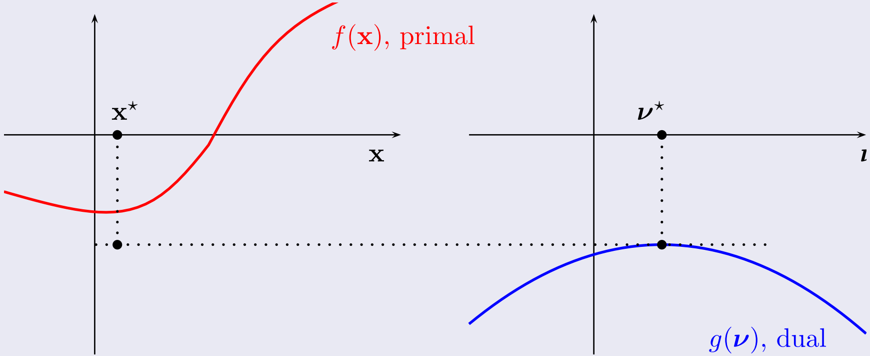
  making no assumption of f, g and h.

- Let us denote by f^* the optimal value of the decision function under the constraints, i.e., $f^* = f\left(x^*\right)$ if the minimum is reached at a global minimum x^*.

Duality

Duality provides of a concave *dual* function q from a *primal* function f such that for all pair x, ν, the value $f(x)$ is greater than $q(\nu)$.

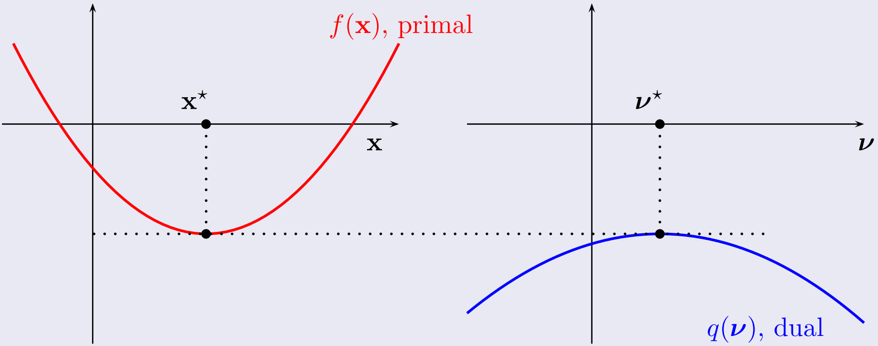
Weak Duality



Duality

For most "reasonable" convex problems, duality comes with an additional property called strong duality, which is very useful.

Strong Duality

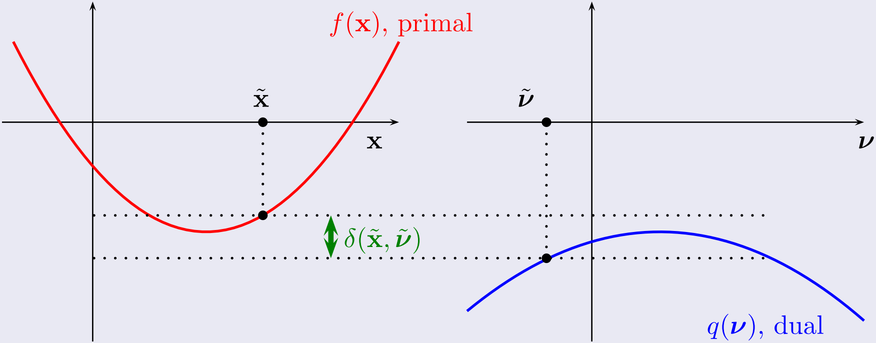


- Strong duality means that $\max_{\boldsymbol{\nu}} q(\boldsymbol{\nu}) = \min_{\mathbf{x}} f(\mathbf{x})$

Duality

For instance, we have the concept of duality gap, which are very useful to stop an optimization algorithm.

Duality gaps



- The duality gap guarantees us that $0 \leq f(\tilde{\mathbf{x}}) - f(\mathbf{x}^\star) \leq \delta(\tilde{\mathbf{x}}, \tilde{\boldsymbol{\nu}})$.
- Dual problems are often obtained by Lagrangian or Fenchel duality.

Optimization problems

Setting

- We consider an equality and inequality constrained optimization problem over a variable $x \in \mathcal{X}$:

$$
\begin{aligned}
\text{minimize} \quad & f(x) \\
\text{subject to} \quad & h_i(x) = 0\,, \quad i = 1, \ldots, m\,, \\
& g_j(x) \leq 0\,, \quad j = 1, \ldots, r\,,
\end{aligned}
$$

  making no assumption of f, g and h.
- Let us denote by f^* the optimal value of the decision function under the constraints, i.e., $f^* = f\left(x^*\right)$ if the minimum is reached at a global minimum x^*.

Lagrangian and dual function

Lagrangian

The Lagrangian of this problem is the function $L : \mathcal{X} \times \mathbb{R}^m \times \mathbb{R}^r \to \mathbb{R}$ defined by:

$$L(x, \lambda, \mu) = f(x) + \sum_{i=1}^{m} \lambda_i h_i(x) + \sum_{j=1}^{r} \mu_j g_j(x) .$$

Lagrangian dual function

The Lagrange dual function $g : \mathbb{R}^m \times \mathbb{R}^r \to \mathbb{R}$ is:

$$\begin{aligned} q(\lambda, \mu) &= \inf_{x \in \mathcal{X}} L(x, \lambda, \mu) \\ &= \inf_{x \in \mathcal{X}} \left(f(x) + \sum_{i=1}^{m} \lambda_i h_i(x) + \sum_{j=1}^{r} \mu_j g_j(x) \right) . \end{aligned}$$

Properties of the dual function

- q is concave in (λ, μ), even if the original problem is not convex.
- The dual function yields lower bounds on the optimal value f^* of the original problem when μ is nonnegative:

$$q(\lambda, \mu) \leq f^* \;, \quad \forall \lambda \in \mathbb{R}^m, \forall \mu \in \mathbb{R}^r, \mu \geq 0 \;.$$

Proofs

- For each x, the function $(\lambda, \mu) \mapsto L(x, \lambda, \mu)$ is linear, and therefore both convex and concave in (λ, μ). The pointwise minimum of concave functions is concave, therefore q is concave.
- Let $\bar{x}$ be any feasible point, i.e., $h(\bar{x}) = 0$ and $g(\bar{x}) \leq 0$. Then we have, for any λ and $\mu \geq 0$:

$$\sum_{i=1}^{m} \lambda_i h_i(\bar{x}) + \sum_{i=1}^{r} \mu_i g_i(\bar{x}) \leq 0 \, ,$$

$$\Longrightarrow \quad L(\bar{x}, \lambda, \mu) = f(\bar{x}) + \sum_{i=1}^{m} \lambda_i h_i(\bar{x}) + \sum_{i=1}^{r} \mu_i g_i(\bar{x}) \leq f(\bar{x}) \, ,$$

$$\Longrightarrow \quad q(\lambda, \mu) = \inf_x L(x, \lambda, \mu) \leq L(\bar{x}, \lambda, \mu) \leq f(\bar{x}) \, , \quad \forall \bar{x} \, . \quad \square$$

Dual problem

Definition

For the (primal) problem:

$$\begin{aligned} \text{minimize} \quad & f(x) \\ \text{subject to} \quad & h(x) = 0 \, , \quad g(x) \leq 0 \, , \end{aligned}$$

the Lagrange dual problem is:

$$\begin{aligned} \text{maximize} \quad & q(\lambda, \mu) \\ \text{subject to} \quad & \mu \geq 0 \, , \end{aligned}$$

where q is the (concave) Lagrange dual function and λ and μ are the Lagrange multipliers associated to the constraints $h(x) = 0$ and $g(x) \leq 0$.

Weak duality

- Let d^* the optimal value of the Lagrange dual problem. Each $q(\lambda, \mu)$ is an lower bound for f^* and by definition d^* is the best lower bound that is obtained. The following weak duality inequality therefore always hold:

$$d^* \leq f^* \; .$$

- This inequality holds when d^* or f^* are infinite. The difference $d^* - f^*$ is called the optimal duality gap of the original problem.

Strong duality

- We say that strong duality holds if the optimal duality gap is zero, i.e.:

$$d^* = f^* \; .$$

- If strong duality holds, then the best lower bound that can be obtained from the Lagrange dual function is tight
- Strong duality does not hold for general nonlinear problems.
- It usually holds for convex problems.
- Conditions that ensure strong duality for convex problems are called constraint qualification.

Slater's constraint qualification

Strong duality holds for a convex problem:

$$\begin{aligned} \text{minimize} \quad & f(x) \\ \text{subject to} \quad & g_j(x) \leq 0 \,, \quad j = 1, \ldots, r \,, \\ & Ax = b \,, \end{aligned}$$

if it is strictly feasible, i.e., there exists at least one feasible point that satisfies:

$$g_j(x) < 0 \,, \quad j = 1, \ldots, r \,, \quad Ax = b \,.$$

Remarks

- Slater's conditions also ensure that the maximum d^* (if $> -\infty$) is attained, i.e., there exists a point (λ^*, μ^*) with

$$q(\lambda^*, \mu^*) = d^* = f^*$$

- They can be sharpened. For example, strict feasibility is not required for affine constraints.
- There exist many other types of constraint qualifications

Dual optimal pairs

Suppose that strong duality holds, x^* is primal optimal, (λ^*, μ^*) is dual optimal. Then we have:

$$
\begin{aligned}
f(x^*) &= q\left(\lambda^*, \mu^*\right) \\
&= \inf_{x \in \mathbb{R}^n} \left\{ f(x) + \sum_{i=1}^{m} \lambda_i^* h_i(x) + \sum_{j=1}^{r} \mu_j^* g_j(x) \right\} \\
&\leq f(x^*) + \sum_{i=1}^{m} \lambda_i^* h_i(x^*) + \sum_{j=1}^{r} \mu_j^* g_j(x^*) \\
&\leq f(x^*)
\end{aligned}
$$

Hence both inequalities are in fact equalities.

Complimentary slackness

The first equality shows that:

$$L\left(x^*, \lambda^*, \mu^*\right) = \inf_{x \in \mathbb{R}^n} L\left(x, \lambda^*, \mu^*\right) \ ,$$

showing that x^* minimizes the Lagrangian at (λ^*, μ^*). The second equality shows that:

$$\mu_j g_j(x^*) = 0 \ , \quad j = 1, \ldots, r \ .$$

This property is called complementary slackness:
the ith optimal Lagrange multiplier is zero unless the ith constraint is active at the optimum.

Outline

Lagrangian

In order to minimize:

$$\frac{1}{2}\| w \|^2$$

under the constraints:

$$\forall i = 1, \ldots, n\,, \qquad y_i\left(w^\top x_i + b\right) - 1 \geq 0\,,$$

we introduce one dual variable α_i for each constraint, i.e., for each training point. The Lagrangian is:

$$L(w, b, \alpha) = \frac{1}{2}||w||^2 - \sum_{i=1}^{n} \alpha_i \left(y_i\left(w^\top x_i + b\right) - 1\right)\,.$$

Lagrangian

- $L\left(w,b,\alpha\right)$ is convex quadratic in w. It is minimize for:

$$\nabla_w L = w - \sum_{i=1}^{n} \alpha_i y_i x_i = 0 \quad \Longrightarrow \quad w = \sum_{i=1}^{n} \alpha_i y_i x_i \,.$$

- $L\left(w,b,\alpha\right)$ is affine in b. Its minimum is $-\infty$ except if:

$$\nabla_b L = \sum_{i=1}^{n} \alpha_i y_i = 0 \,.$$

Dual function

- We therefore obtain the Lagrange dual function:

$$
\begin{aligned}
q(\alpha) &= \inf_{w \in \mathbb{R}^p, b \in \mathbb{R}} L(w, b, \alpha) \\
&= \begin{cases} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n y_i y_j \alpha_i \alpha_j x_i . x_j & \text{if } \sum_{i=1}^n \alpha_i y_i = 0\,, \\ -\infty & \text{otherwise.} \end{cases}
\end{aligned}
$$

- The dual problem is:

$$
\begin{aligned}
\text{maximize} \quad & q(\alpha) \\
\text{subject to} \quad & \alpha \geq 0\,.
\end{aligned}
$$

Dual problem

Find $\alpha^* \in \mathbb{R}^n$ which maximizes

$$L(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j x_i^\top x_j,$$

under the (simple) constraints $\alpha_i \geq 0$ (for $i = 1, \ldots, n$), and

$$\sum_{i=1}^{n} \alpha_i y_i = 0.$$

This is a quadratic program on $\mathbb{R}^N$, with "box constraints". α^* can be found efficiently using dedicated optimization softwares.

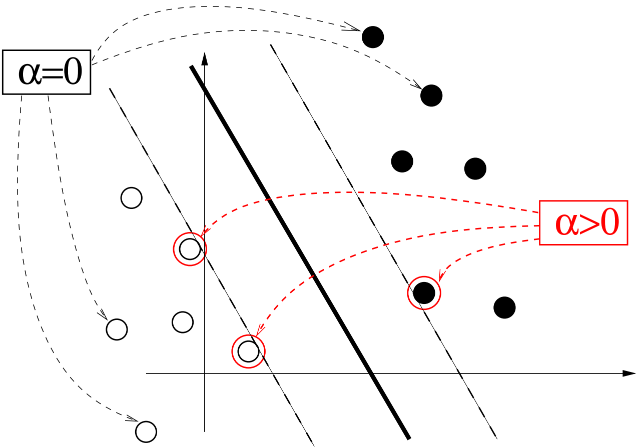
Complementary slackness conditions

- At the optimal, the complementary slackness conditions must hold:

$$\forall i = 1, \ldots, n \quad \alpha_i^* \left(y_i \left(w^{*\top} x_i + b^* \right) - 1 \right) = 0 \,.$$

- This implies that:
  - If $\alpha_i^* > 0$ then $y_i \left(w^{*\top} x_i + b^* \right) = 1$
  - If $y_i \left(w^{*\top} x_i + b^* \right) > 1$ then $\alpha_i^* = 0$

Interpretation: support vectors



Recovering the optimal hyperplane

- Once α^* is found, we recover w^* by:

$$w^* = \operatorname*{argmin}_w L(w, b, \alpha^*) = \sum_{i=1}^{n} \alpha_i y_i x_i$$

- To recover b we can not just minimize $L(w, b, \alpha^*)$, since it does not depend on b. Instead, we use the complementary slackness condition: if i is such that $\alpha_i > 0$, then

$$y_i \left({w^*}^\top x_i + b^* \right) = 1 \quad \Longrightarrow \quad b^* = y_i - {w^*}^\top x_i$$

- The decision function is therefore:

$$\begin{aligned} f^*(x) &= {w^*}^\top x + b^* \\ &= \sum_{i=1}^{n} \alpha_i y_i x_i^\top x + b^* . \end{aligned}$$

Primal (for large n) vs dual (for large p) optimization

1. Find $(w, b) \in \mathbb{R}^{p+1}$ which minimize:

$$\frac{1}{2}\| w \|^2$$

   under the constraints:

$$\forall i = 1, \ldots, n\,, \qquad y_i \left(w^\top x_i + b \right) - 1 \geq 0\,.$$

2. Find $\alpha^* \in \mathbb{R}^n$ which maximizes

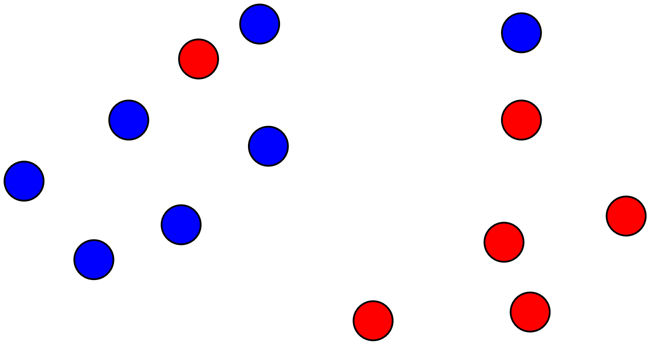
$$L(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j x_i . x_j\,,$$

   under the (simple) constraints $\alpha_i \geq 0$ (for $i = 1, \ldots, n$), and

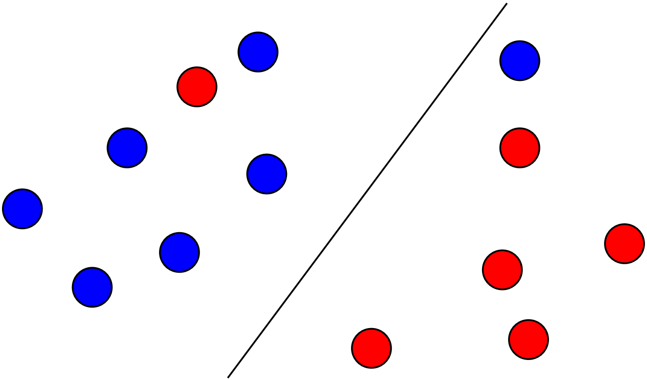
$$\sum_{i=1}^{n} \alpha_i y_i = 0.$$

Outline

What if data are not linearly separable?



What if data are not linearly separable?



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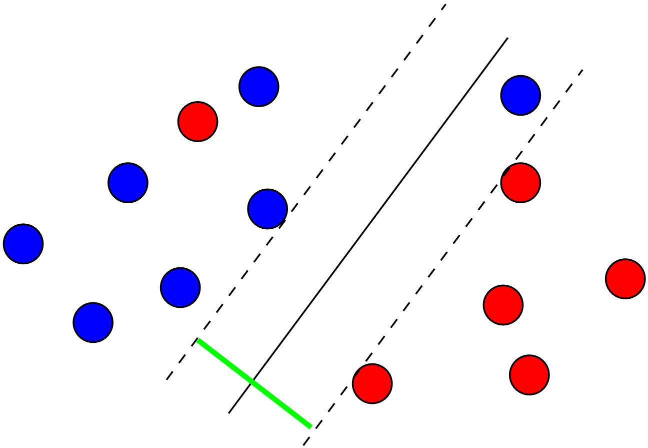

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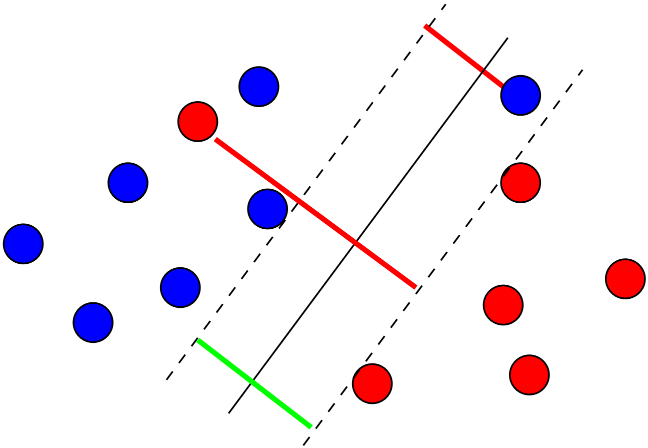
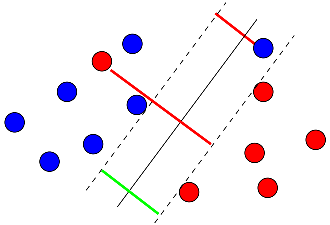


Soft-margin SVM

- Find a trade-off between large margin and few errors.
- Mathematically:

$$\min_f \left\{ \frac{1}{margin(f)} + C \times errors(f) \right\}$$

- C is a parameter



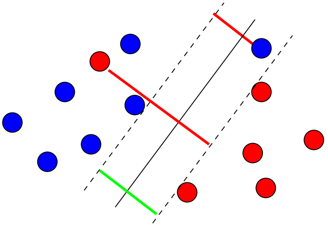
Soft-margin SVM formulation

- The margin of a labeled point (x, y) is

$$margin(x, y) = y \left(w^\top x + b \right)$$

- The error is
  - 0 if $margin(x, y) > 1$,
  - $1 - margin(x, y)$ otherwise.
- The soft margin SVM solves:

$$\min_{w,b} \left\{ \frac{1}{2}||w||^2 + C \sum_{i=1}^{n} \max \left(0, 1 - y_i \left(w^\top x_i + b \right) \right) \right\}$$

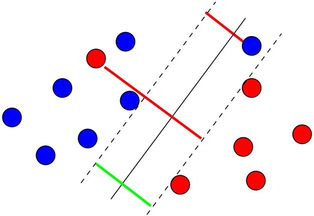


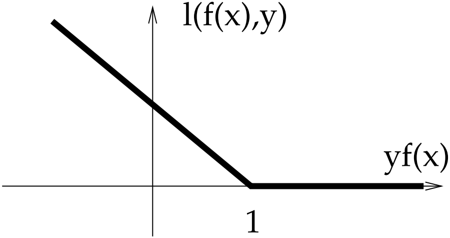
Soft-margin SVM and hinge loss

$$\min_{w,b} \left\{ \frac{1}{n} \sum_{i=1}^{n} \ell_{\text{hinge}} \left(w^\top x_i + b, y_i \right) + \lambda \| w \|^2 \right\} ,$$

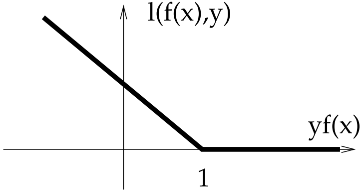
for $\lambda = 1/2nC$ and the hinge loss function:

$$\ell_{\text{hinge}}(u, y) = \max\left(1 - yu, 0\right) = \begin{cases} 0 & \text{if } yu \geq 1, \\ 1 - yu & \text{otherwise.} \end{cases}$$





Reformulation as a QP



- Note that for any $u \in \mathbb{R}$,

$$\varphi_{\text{hinge}}(u) = \min_{\xi \in \mathbb{R}} \xi \quad \text{such that} \quad \begin{cases} \xi \geq 0 \\ \xi \geq 1 - u \end{cases}$$

- Therefore SVM solves the QP

$$\min_{w,b,\xi} \left\{ \frac{1}{2} \| w \|^2 + C \sum_{i=1}^{n} \xi_i \right\}, \text{ s.t. } \forall i \in [1, n], \begin{cases} \xi_i \geq 0 \\ \xi_i \geq 1 - y_i \left(w^\top x_i + b \right) \end{cases}$$

Lagrangian

Form the Lagrangian:

$$L(w, b, \xi, \alpha, \gamma) = \frac{1}{2}\| w \|^2 + C \sum_{i=1}^{n} \xi_i - \sum_{i=1}^{n} \alpha_i \left(y_i x_i^\top w + \xi_i - 1 \right) - \gamma^\top \xi$$

Minimize in the primal variables (w, b, ξ):

$$\nabla_w L = w - \sum_{i=1}^{n} \alpha_i y_i x_i \quad \Longrightarrow \quad w = \sum_{i=1}^{n} \alpha_i y_i x_i$$

$$\nabla_{\xi_i} L = C - \alpha_i - \gamma_i \quad \Longrightarrow \quad \alpha_i + \gamma_i = C$$

Dual formulation

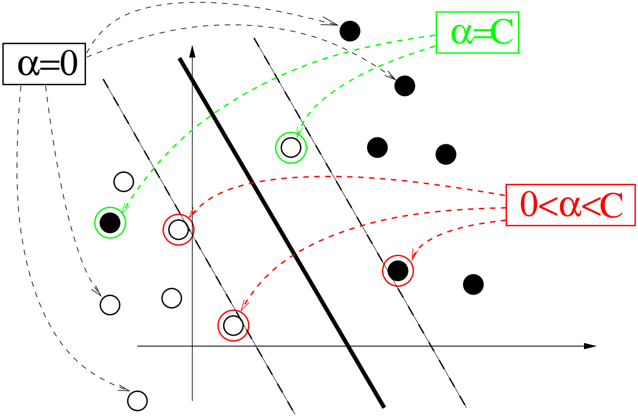
$$\max_{\alpha \in \mathbb{R}^n} \left\{ \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j x_i^\top x_j \right\}$$

under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C\,, & \text{for } i = 1, \ldots, n \\ \sum_{i=1}^{n} \alpha_i y_i = 0\,. \end{cases}$$

Remark: we recover hard-margin SVM with $C = +\infty$

Interpretation: bounded and unbounded support vectors



Outline

Loss functions for classifications

We already saw 3 loss functions for binary classification problems

- The 0/1 loss $\ell_{0/1}(f(x), y) = \mathbf{1}(yf(x) < 0)$
- The logistic loss $\ell_{logistic}(f(x), y) = \ln\left(1 + e^{-yf(x)}\right)$
- The hinge loss $\ell_{hinge}(f(x), y) = \max(0, 1 - yf(x))$

Definition

In binary classification ($\mathcal{Y} = \{-1, 1\}$), the margin of the function f for a pair (x, y) is:

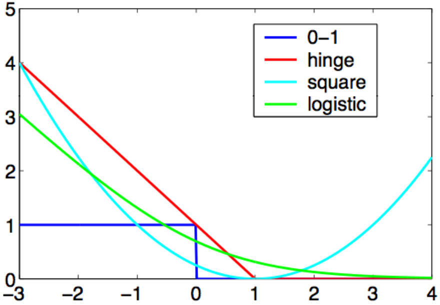
$$yf(x).$$

In all cases the loss is a decreasing function of the margin, i.e.,

$$\ell(f(x), y) = \varphi(yf(x)), \quad \text{with } \varphi \text{ non-increasing}$$

What about other similar loss functions?

Loss function examples



Method	$\varphi(u)$
Logistic regression	$\log\left(1+e^{-u}\right)$
Support vector machine (1-SVM)	$\max\left(1-u,0\right)$
Support vector machine (2-SVM)	$\max\left(1-u,0\right)^2$
Boosting	e^{-u}

Large-margin classifiers

Definition

Given a non-increasing function $\varphi : \mathbb{R} \to \mathbb{R}_+$, a large-margin linear classifier is an algorithm that estimates a function $f_\beta(x) = \beta^\top x$ by solving

$$\min_\beta \frac{1}{n} \sum_{i=1}^{n} \varphi\left(y_i f_\beta(x_i)\right) + \lambda \| \beta \|_2^2$$

Hence, ridge logistic regression and SVM are large-margin classifier, corresponding to $\varphi(u) = \ln\left(1 + e^{-u}\right)$ and $\varphi(u) = \max(0, 1 - u)$, respectively. Many more are possible.

Questions:

1. Can we solve the optimization problem for other φ's?
2. Is it a good idea to optimize this objective function, if at the end of the day we are interested in the $\ell_{0/1}$ loss, i.e., learning models that make few errors?

Solving large-margin classifiers

$$\min_{\beta} \frac{1}{n} \sum_{i=1}^{n} \varphi\left(y_i \beta^\top x_i\right) + \lambda \| \beta \|_2^2$$

- When φ is convex, this is a stricly convex function of β
- It can then be solved numerically by generic or specific algorithms for convex optimization, e.g., Newton's or gradient method
- When n is large, stochastic optimization is particularly useful (at each step, only approximate the gradient with one or a batch of examples)

A tiny bit of learning theory

Assumptions and notations

- Let $\mathbb{P}$ be an (unknown) distribution on $\mathcal{X} \times \mathcal{Y}$, and $\eta(x) = \mathbb{P}(Y = 1 \,|\, X = x)$ a measurable version of the conditional distribution of Y given X
- Assume the training set $\mathcal{S}_n = (X_i, Y_i)_{i=1,\dots,n}$ are i.i.d. random variables according to $\mathbb{P}$.
- The risk of a classifier $f : \mathcal{X} \to \mathbb{R}$ is $R(f) = \mathbb{P}\left(sign(f(X)) \neq Y\right)$
- The Bayes risk is

$$R^* = \inf_{f \text{ measurable}} R(f)$$

  which is attained for $f^*(x) = \eta(x) - 1/2$
- The empirical risk of a classifier $f : \mathcal{X} \to \mathbb{R}$ is

$$R^n(f) = \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}\left(sign(f(X_i)) \neq Y_i\right)$$

φ-risk

- Let the empirical φ-risk be the empirical risk optimized by a large-margin classifier:

$$R_\varphi^n(f) = \frac{1}{n}\sum_{i=1}^{n} \varphi\left(Y_i f(X_i)\right)$$

- It is the empirical version of the φ-risk

$$R_\varphi(f) = \mathbb{E}[\varphi\left(Yf\left(X\right)\right)]$$

- Can we hope to have a small risk $R(f)$ if we focus instead on the φ-risk $R_\varphi(f)$?

A small φ-risk ensures a small $0/1$ risk

Theorem (Bartlett et al., 2003)

Let $\varphi : \mathbb{R} \to \mathbb{R}_+$ be convex, non-increasing, differentiable at 0 with $\varphi'(0) < 0$. Let $f : \mathcal{X} \to \mathbb{R}$ measurable such that

$$R_\varphi(f) = \min_{g \text{ measurable}} R_\varphi(g) = R_\varphi^* .$$

Then

$$R(f) = \min_{g \text{ measurable}} R(g) = R^* .$$

Remarks:

- This tells us that, if we know $\mathbb{P}$, then minimizing the φ-risk is a good idea even if our focus is on the classification error.
- The assumptions on φ can be relaxed; it works for the broader class of *classification-calibrated* loss functions (Bartlett et al., 2003).
- More generally, we can show that if $R_\varphi(f) - R_\varphi^*$ is small, then $R(f) - R^*$ is small too (Bartlett et al., 2003).

A small φ-risk ensures a small 0/1 risk

Proof sketch:
Condition on $X = x$:

$$R_\varphi(f \mid X = x) = \mathbb{E}\left[\varphi\left(Yf\left(X\right)\right) \mid X = x\right] = \eta(x)\varphi\left(f(x)\right) + (1 - \eta(x))\,\varphi\left(-f(x)\right)$$
$$R_\varphi(-f \mid X = x) = \mathbb{E}\left[\varphi\left(-Yf\left(X\right)\right) \mid X = x\right] = \eta(x)\varphi\left(-f(x)\right) + (1 - \eta(x))\,\varphi\left(f(x)\right)$$

Therefore:

$$R_\varphi(f \mid X = x) - R_\varphi(-f \mid X = x) = [2\eta(x) - 1] \times \left[\varphi\left(f(x)\right) - \varphi\left(-f(x)\right)\right]$$

This must be a.s. ≤ 0 because $R_\varphi(f) \leq R_\varphi(-f)$, which implies:

- if $\eta(x) > \frac{1}{2}$, $\varphi\left(f(x)\right) \leq \varphi\left(-f(x)\right) \implies f(x) \geq 0$
- if $\eta(x) < \frac{1}{2}$, $\varphi\left(f(x)\right) \geq \varphi\left(-f(x)\right) \implies f(x) \leq 0$

These inequalities are in fact strict thanks to the assumptions we made on φ (*left as exercice*). $\square$

Empirical risk minimization (ERM)

To find a function with a small φ-risk, the following is a good candidate:

Definition

The ERM estimator on a functional class $\mathcal{F}$ is the solution (when it exists) of:

$$\hat{f}_n = \operatorname*{argmin}_{f \in \mathcal{F}} R_\varphi^n(f)\,.$$

Empirical risk minimization (ERM)

To find a function with a small φ-risk, the following is a good candidate:

Definition

The ERM estimator on a functional class $\mathcal{F}$ is the solution (when it exists) of:

$$\hat{f}_n = \operatorname*{argmin}_{f \in \mathcal{F}} R^n_\varphi(f)\,.$$

Questions:

1. Is $R^n_\varphi(f)$ a good estimate of the true risk $R_\varphi(f)$?
2. Is $R_\varphi(\hat{f}_n)$ small?

Class capacity

Motivations

- The ERM principle gives a good solution if $R_\varphi\left(\hat{f}_n\right)$ is similar to the minimum achievable risk $\inf_{f\in\mathcal{F}} R_\varphi(f)$.
- This can be ensured if $\mathcal{F}$ is not "too large".
- We need a measure of the "capacity" of $\mathcal{F}$.

Definition: Rademacher complexity

The Rademacher complexity of a class of functions $\mathcal{F}$ is:

$$\mathrm{Rad}_n\left(\mathcal{F}\right) = \mathbb{E}_{X,\sigma}\left[\sup_{f\in\mathcal{F}}\left|\frac{2}{n}\sum_{i=1}^{n}\sigma_i f\left(X_i\right)\right|\right],$$

where the expectation is over $(X_i)_{i=1,\ldots,n}$ and the independent uniform $\{\pm 1\}$-valued (Rademacher) random variables $(\sigma_i)_{i=1,\ldots,n}$.

Basic learning bounds

Theorem

Suppose φ is Lipschitz with constant L_φ:

$$\forall u, u' \in \mathbb{R}, \quad \left| \varphi(u) - \varphi(u') \right| \leq L_\varphi \left| u - u' \right| .$$

Then the φ-risk of the ERM estimator satisfies (on average over the sampling of training set)

$$\underbrace{\mathbb{E}_{\mathcal{S}_n} R_\varphi\left(\hat{f}_n\right) - R_\varphi^*}_{\text{Excess } \varphi\text{-risk}} \leq \underbrace{4 L_\varphi \mathrm{Rad}_n\left(\mathcal{F}\right)}_{\text{Estimation error}} + \underbrace{\inf_{f \in \mathcal{F}} R_\varphi(f) - R_\varphi^*}_{\text{Approximation error}}$$

This quantifies a trade-off between:

- $\mathcal{F}$ "large" $=$ overfitting (approximation error small, estimation error large)
- $\mathcal{F}$ "small" $=$ underfitting (estimation error small, approximation error large)

ERM for bounded linear classifiers

Consider the set of linear functions $f_\beta(x) = \beta^\top x$ where β is bounded:

$$\mathcal{F}_B = \{f_\beta : \|\beta\|_2 \leq B\} .$$

Theorem

$$\mathrm{Rad}_n(\mathcal{F}_B) \leq \frac{2B\sqrt{\mathbb{E}\|X\|_2^2}}{\sqrt{n}} .$$

Proof (1/2)

$$
\begin{aligned}
\mathrm{Rad}_n(\mathcal{F}_B) &= \mathbb{E}_{X,\sigma}\left[\sup_{f\in\mathcal{F}_B}\left|\frac{2}{n}\sum_{i=1}^{n}\sigma_i f(X_i)\right|\right] \\
&= \mathbb{E}_{X,\sigma}\left[\sup_{\|\beta\|\leq B}\left|\left\langle \beta, \frac{2}{n}\sum_{i=1}^{n}\sigma_i X_i\right\rangle\right|\right] \quad \text{(linearity)} \\
&= \mathbb{E}_{X,\sigma}\left[B\left\|\frac{2}{n}\sum_{i=1}^{n}\sigma_i X_i\right\|_2\right] \quad \text{(Cauchy-Schwarz)} \\
&= \frac{2B}{n}\mathbb{E}_{X,\sigma}\left[\sqrt{\left\|\sum_{i=1}^{n}\sigma_i X_i\right\|_2^2}\right] \\
&\leq \frac{2B}{n}\sqrt{\mathbb{E}_{X,\sigma}\left[\sum_{i,j=1}^{n}\sigma_i\sigma_j X_i^\top X_j\right]} \quad \text{(Jensen)}
\end{aligned}
$$

Proof (2/2)

But $\mathbb{E}_\sigma [\sigma_i \sigma_j]$ is 1 if $i = j$, 0 otherwise. Therefore:

$$\begin{aligned} \mathrm{Rad}_n(\mathcal{F}_B) &\leq \frac{2B}{n} \sqrt{\mathbb{E}_X \left[\sum_{i,j=1}^{n} \mathbb{E}_\sigma [\sigma_i \sigma_j] X_i^\top X_j \right]} \\ &\leq \frac{2B}{n} \sqrt{\mathbb{E}_X \sum_{i=1}^{n} \| X_i \|_2^2} \\ &= \frac{2B \sqrt{\mathbb{E}_X \| X \|_2^2}}{\sqrt{n}} . \quad \square \end{aligned}$$

Basic learning bounds in RKHS balls

Corollary

Suppose $\| X \| \leq \kappa$ a.s. Then the ERM estimator in $\mathcal{F}_B$ satisfies

$$\mathbb{E}R_\varphi\left(\hat{f}_n\right) - R^*_\varphi \leq \frac{8L_\varphi \kappa B}{\sqrt{n}} + \left[\inf_{f\in\mathcal{F}_B} R_\varphi(f) - R^*_\varphi\right].$$

Remarks

- B controls the trade-off between approximation and estimation error
- The bound on expression error is independent of $\mathcal{P}$ and decreases with n
- The approximation error is harder to analyze in general
- In practice, B (or λ, next slide) is tuned by cross-validation

ERM as penalized risk minimization

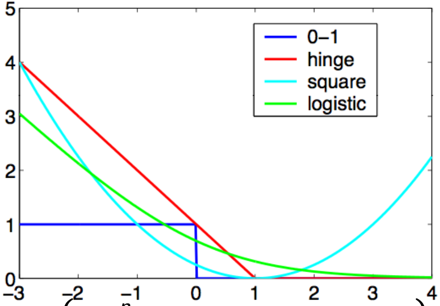
- ERM over $\mathcal{F}_B$ solves the constrained minimization problem:

$$\begin{cases} \min_\beta \frac{1}{n} \sum_{i=1}^{n} \varphi\left(y_i f_\beta\left(x_i\right)\right) \\ \text{subject to } \| \beta \|_2 \leq B \,. \end{cases}$$

- To make this practical we assume that φ is convex.
- The problem is then a convex problem in β for which strong duality holds. In particular β solves the problem if and only if it solves for some dual parameter λ the unconstrained problem:

$$\min_{\beta \in \mathbb{R}^p} \left\{ \frac{1}{n} \sum_{i=1}^{n} \varphi\left(y_i f_\beta\left(x_i\right)\right) + \lambda \| \beta \|_2^2 \right\} .$$

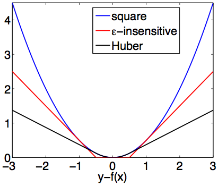
Summary: large margin classifiers

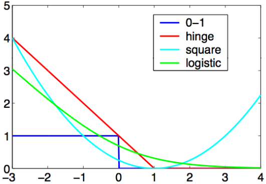


$$\min_{f \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \varphi \left(y_i f \left(x_i \right) \right) + \lambda \| f \|_{\mathcal{H}}^2 \right\}$$

- φ calibrated (e.g., decreasing, $\varphi'(0) < 0$) $\implies$ good proxy for classification error
- φ convex + representer theorem $\implies$ efficient algorithms

Summary: ℓ_2-regularized linear methods



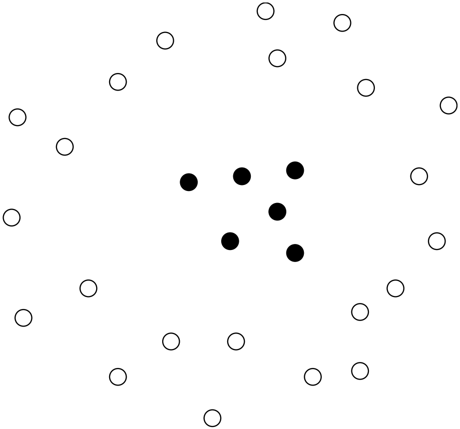


$$f_\beta(x) = \beta^\top x\,, \quad \min_\beta \left\{ \frac{1}{n}\sum_{i=1}^{n} \ell(f_\beta(x_i), y_i) + \lambda \|\beta\|_2^2 \right\}$$

- Many popular methods for regression and classification are obtained by changing the loss function: ridge regression, logistic regression, SVM...
- Needs to solve numerically a convex optimization problem, well adapted to large datasets (stochastic gradient...)
- In practice, very similar performance between the different variants in general

Outline

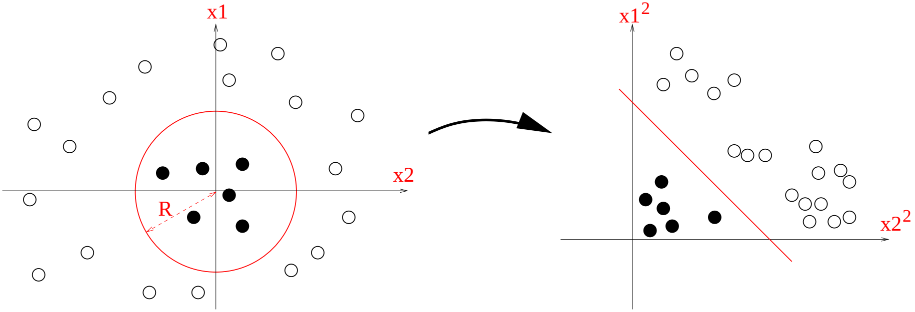
Motivation



- Sometimes linear models are not interesting...
- Kernels will allow to solve nonlinear problems with linear methods!

Outline

"Linear" depends on the representation you choose



For $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ let $\Phi(x) = \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix}$. The decision function is:

$$f(x) = x_1^2 + x_2^2 - R^2 = \color{red}{\beta^\top \Phi(x) + b}$$

with $\beta = (1,1)^\top$ and $b = -R^2$

Kernel = inner product in the feature space

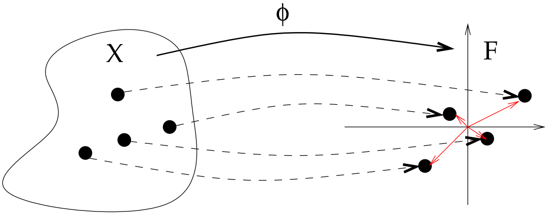
Definition

For a given mapping

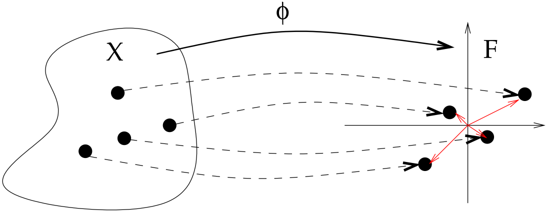
$$\Phi : \mathcal{X} \mapsto \mathcal{H}$$

from the space of data $\mathcal{X}$ to some feature space $\mathcal{H}$, the kernel between two objects x and x' is the inner product of their images:

$$\forall x, x' \in \mathcal{X}, \quad K(x, x') = \Phi(x)^\top \Phi(x') \, .$$



Example

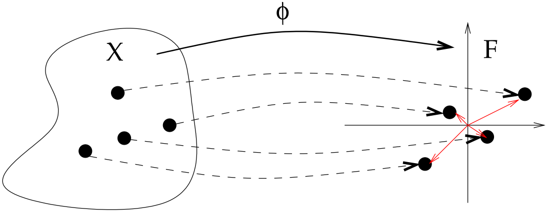


Let $\mathcal{X} = \mathcal{H} = \mathbb{R}^2$ and for $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ let $\Phi(x) = \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix}$

Then the kernel is:

$$K(x, x') = \Phi(x)^\top \Phi(x') = (x_1)^2 (x_1')^2 + (x_2)^2 (x_2')^2 \,.$$

The kernel tricks



2 tricks

1. Many linear algorithms (in particular ℓ_2-regularized methods) can be performed in the feature space of $\Phi(x)$ without explicitly computing the images $\Phi(x)$, but instead by computing kernels $K(x, x')$.
2. It is sometimes possible to easily compute kernels which correspond to complex large-dimensional feature spaces: $K(x, x')$ is often much simpler to compute than $\Phi(x)$ and $\Phi(x')$

Trick 1 illustration: SVM in the original space

- Train the SVM by maximizing

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^\top \mathbf{x}_j \,,$$

under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C \,, & \text{for } i = 1, \ldots, n \\ \sum_{i=1}^{n} \alpha_i y_i = 0 \,. \end{cases}$$

- Predict with the decision function

$$f(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i^\top \mathbf{x} + b^* \,.$$

Trick 1 illustration: SVM in the feature space

- Train the SVM by maximizing

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \Phi\left(x_i\right)^\top \Phi\left(x_j\right) ,$$

under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C \,, & \text{for } i = 1, \ldots, n \\ \sum_{i=1}^{n} \alpha_i y_i = 0 \,. \end{cases}$$

- Predict with the decision function

$$f\left(x\right) = \sum_{i=1}^{n} \alpha_i y_i \Phi\left(x_i\right)^\top \Phi\left(x\right) + b^* \,.$$

Trick 1 illustration: SVM in the feature space with a kernel

- Train the SVM by maximizing

$$\max_{\alpha\in\mathbb{R}^n} \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i\alpha_j y_i y_j K\left(x_i, x_j\right) ,$$

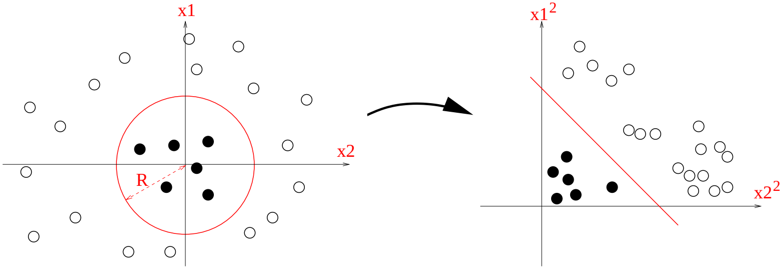
under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C\,, & \text{for } i = 1, \ldots, n \\ \sum_{i=1}^{n} \alpha_i y_i = 0\,. \end{cases}$$

- Predict with the decision function

$$f\left(x\right) = \sum_{i=1}^{n} \alpha_i K\left(x_i, x\right) + b^*\,.$$

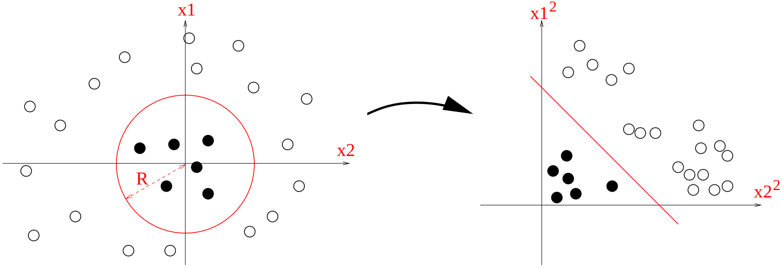
Trick 2 illustration: polynomial kernel



For $x = (x_1, x_2)^\top \in \mathbb{R}^2$, let $\Phi(x) = (x_1^2, \sqrt{2}x_1x_2, x_2^2) \in \mathbb{R}^3$:

$$
\begin{aligned}
K(x, x') &= x_1^2 x_1'^2 + 2x_1x_2x_1'x_2' + x_2^2x_2'^2 \\
&= \left(x_1x_1' + x_2x_2'\right)^2 \\
&= \left(x^\top x'\right)^2 .
\end{aligned}
$$

Trick 2 illustration: polynomial kernel



More generally, for $x, x' \in \mathbb{R}^p$,

$$K(x,x') = \left(x^\top x' + 1\right)^d$$

is an inner product in a feature space of all monomials of degree up to d *(left as exercice.)*

Combining tricks: learn a polynomial discrimination rule with SVM

- Train the SVM by maximizing

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \left(x_i^\top x_j + 1 \right)^d ,$$

under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C \,, & \text{for } i = 1, \ldots, n \\ \sum_{i=1}^{n} \alpha_i y_i = 0 \,. \end{cases}$$

- Predict with the decision function

$$f(x) = \sum_{i=1}^{n} \alpha_i y_i \left(x_i^\top x + 1 \right)^d + b^* \,.$$

Illustration: toy nonlinear problem

```
> plot(x,col=ifelse(y>0,1,2),pch=ifelse(y>0,1,2))
```

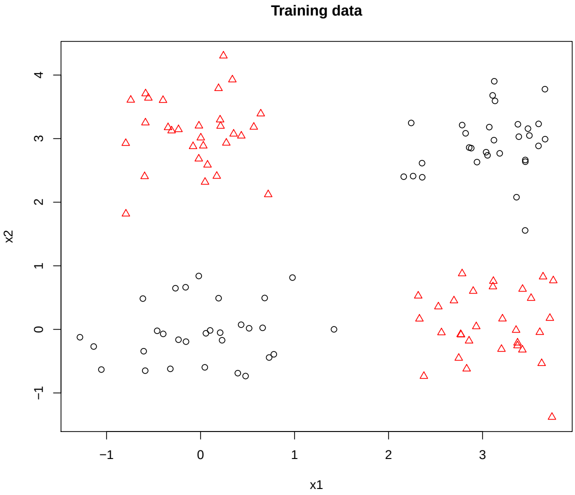


Illustration: toy nonlinear problem, linear SVM

```
> library(kernlab)
> svp <- ksvm(x,y,type="C-svc",kernel='vanilladot')
> plot(svp,data=x)
```

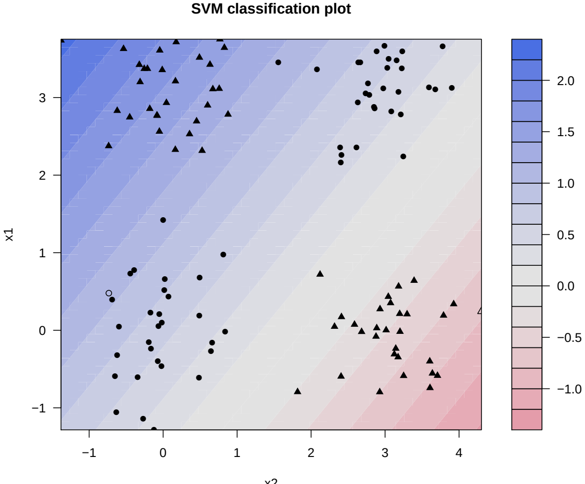
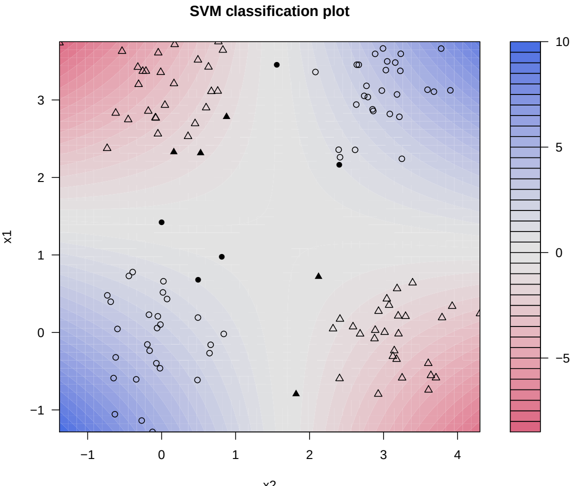


Illustration: toy nonlinear problem, polynomial SVM

```
> svp <- ksvm(x,y,type="C-svc", ...
                              kernel=polydot(degree=2))
> plot(svp,data=x)
```



More generally: trick 1 for ℓ_2-regularized linear models

Representer theorem

Let $f_\beta(x) = \beta^\top \Phi(x)$. Then any solution $\hat{f}_\beta$ of

$$\min_\beta \frac{1}{n} \sum_{i=1}^n \ell(f_\beta(x_i), y_i) + \lambda \|\beta\|_2^2$$

can be expanded as

$$\hat{f}_\beta(x) = \sum_{i=1}^n \alpha_i K(x_i, x)\,,$$

where $\alpha \in \mathbb{R}^n$ is a solution of:

$$\min_{\alpha \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^n \ell\left(\sum_{j=1}^n \alpha_j K(x_i, x_j), y_i\right) + \lambda \sum_{i,j=1}^n \alpha_i \alpha_j K(x_i, x_j)\,.$$

Representer theorem: proof

- For any $\beta \in \mathbb{R}^p$, decompose $\beta = \beta_{\mathcal{S}} + \beta_{\perp}$ where $\beta_{\mathcal{S}} \in span(\Phi(x_1), \ldots, \Phi(x_n))$ and $\beta_{\perp}$ is orthogonal to it.
- On any point x_i of the training set, we have:

$$f_\beta(x_i) = \beta^\top \Phi(x_i) = \beta_{\mathcal{S}}^\top \Phi(x_i) + \beta_{\perp}^\top \Phi(x_i) = \beta_{\mathcal{S}}^\top \Phi(x_i) = f_{\beta_{\mathcal{S}}}(x_i)\,.$$

- On the other hand, we have $\| \beta \|_2^2 = \| \beta_{\mathcal{S}} \|_2^2 + \| \beta_{\perp} \|_2^2 \geq \| \beta_{\mathcal{S}} \|_2^2$, with strict inequality if $\beta_{\perp} \neq 0$.
- Consequently, $\beta_{\mathcal{S}}$ is always as good as β in terms of objective function, and strictly better if $\beta_{\perp} \neq 0$. This implies that at any minimum, $\beta_{\perp} = 0$ and therefore $\beta = \beta_{\mathcal{S}} = \sum_{i=1}^n \alpha_i \Phi(x_i)$ for some $\alpha \in \mathbb{R}^n$.
- We then just replace β by this expression in the objective function, noting that

$$\|\beta\|_2^2 = \| \sum_{i=1}^n \alpha_i \Phi(x_i) \|_2^2 = \sum_{i,j=1}^n \alpha_i \alpha_j \Phi(x_i)^\top \Phi(x_j) = \sum_{i,j=1}^n \alpha_i \alpha_j K(x_i, x_j)\,.$$

Example: kernel ridge regression

- Let $\Phi : \mathcal{X} \to \mathbb{R}^p$ be a feature mapping from the space of data to a Euclidean or Hilbert space.
- Let $f_\beta(x) = \beta^\top \Phi(x)$ and K the corresponding kernel.
- By the representer theorem, any solution of:

$$\hat{f} = \arg\min_{f_\beta} \frac{1}{n} \sum_{i=1}^{n} \left(y_i - f_\beta\left(x_i\right)\right)^2 + \lambda \| \beta \|_2^2$$

can be expanded as:

$$\hat{f} = \sum_{i=1}^{n} \alpha_i K\left(x_i, x\right).$$

Example: kernel ridge regression

- Let $Y = (y_1, \dots, y_n)^\top \in \mathbb{R}^n$ the vector of response variables.
- Let $\alpha = (\alpha_1, \dots, \alpha_n)^\top \in \mathbb{R}^n$ the unknown coefficients.
- Let K be the $n \times n$ Gram matrix: $K_{i,j} = K(x_i, x_j)$.
- We can then write in matrix form:

$$\left(\hat{f}(x_1), \dots, \hat{f}(x_n)\right)^\top = K\alpha,$$

- Moreover,

$$\| \beta \|_2^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j K(x_i, x_j) = \alpha^\top K \alpha.$$

Example: kernel ridge regression

- The problem is therefore equivalent to:

$$\arg\min_{\alpha \in \mathbb{R}^n} \frac{1}{n} (K\alpha - Y)^\top (K\alpha - Y) + \lambda \alpha^\top K \alpha \,.$$

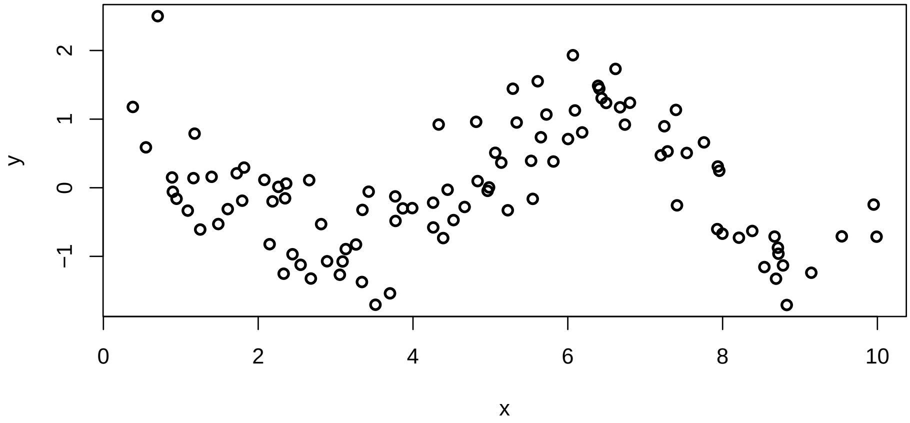
- This is a convex and differentiable function of α. Its minimum can therefore be found by setting the gradient in α to zero:

$$\begin{aligned} 0 &= \frac{2}{n} K (K\alpha - Y) + 2\lambda K \alpha \\ &= K \left[(K + \lambda n I)\, \alpha - Y \right] \end{aligned}$$

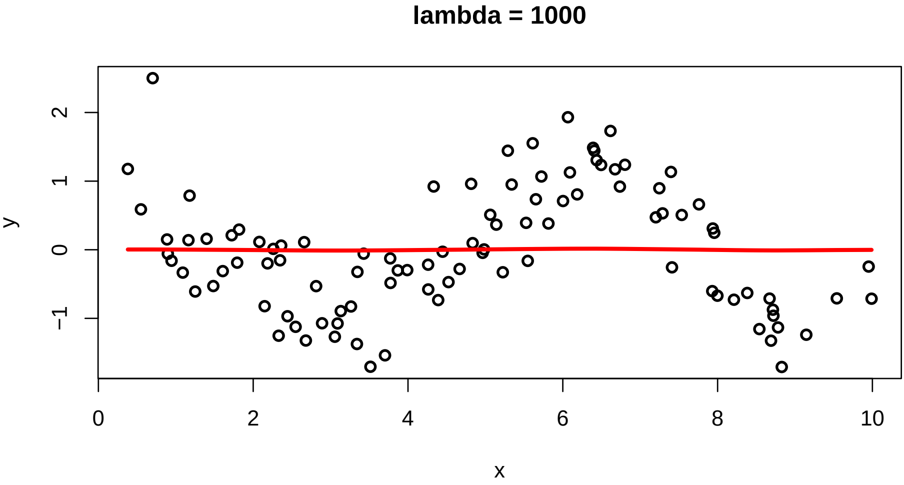
- For $\lambda > 0$, $K + \lambda n I$ is invertible (because K is positive semidefinite) so one solution is to take:

$$\alpha = (K + \lambda n I)^{-1} Y.$$

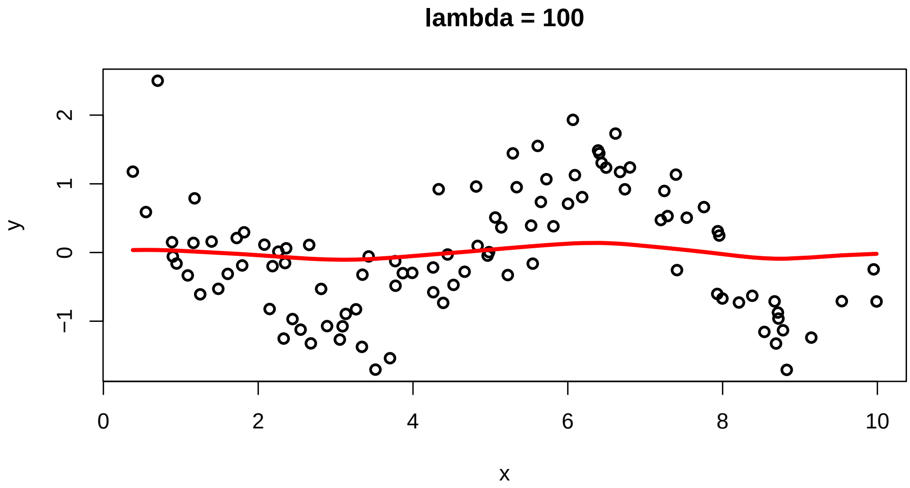
Example (KRR with Gaussian RBF kernel)



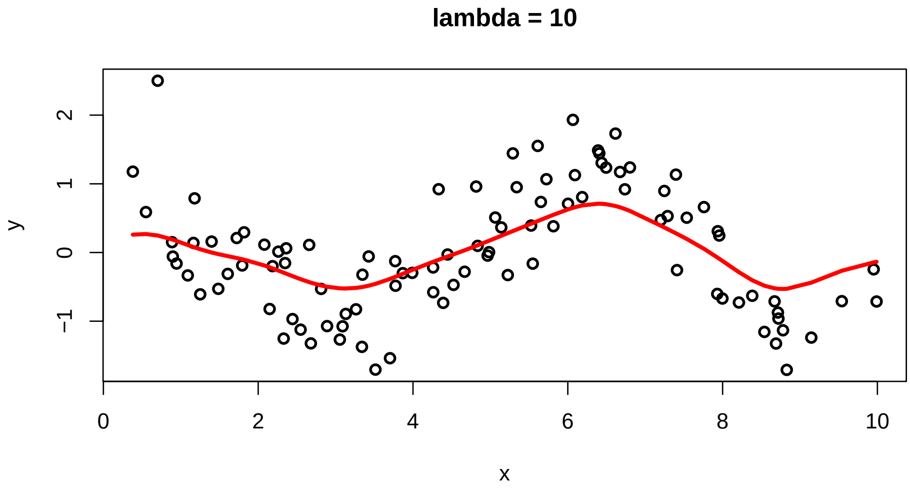
Example (KRR with Gaussian RBF kernel)



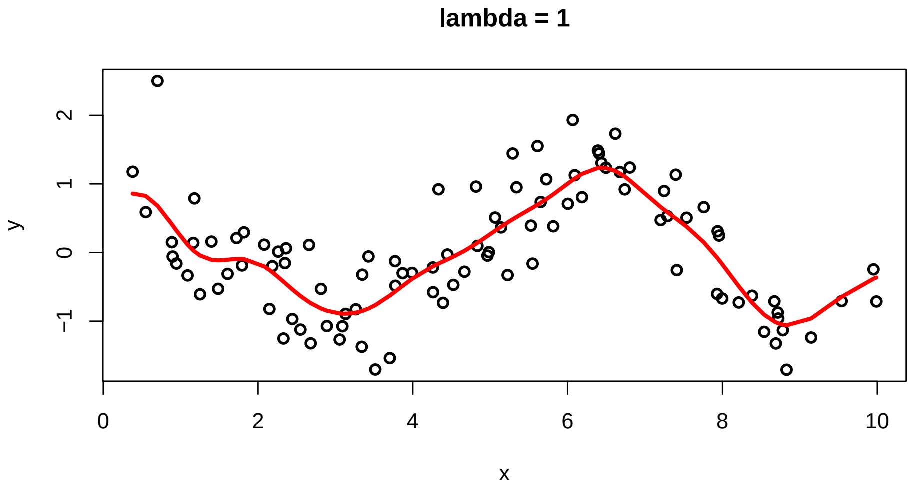
Example (KRR with Gaussian RBF kernel)



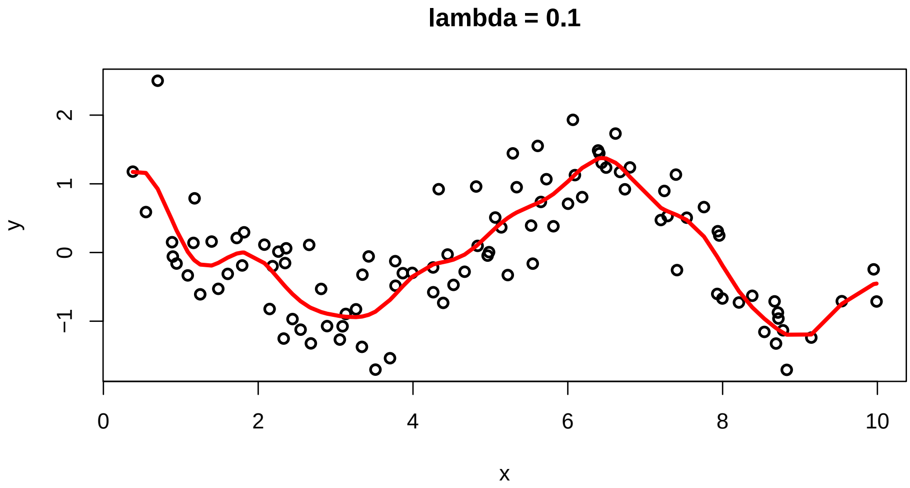
Example (KRR with Gaussian RBF kernel)



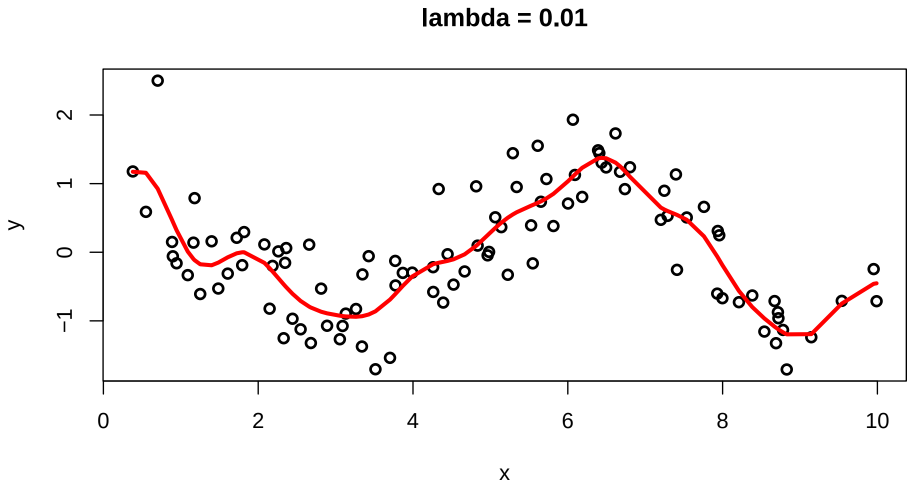
Example (KRR with Gaussian RBF kernel)



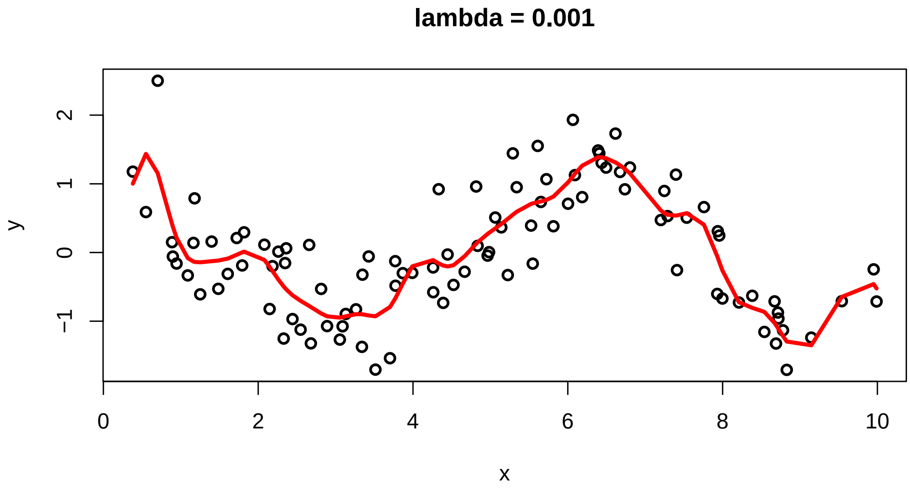
Example (KRR with Gaussian RBF kernel)



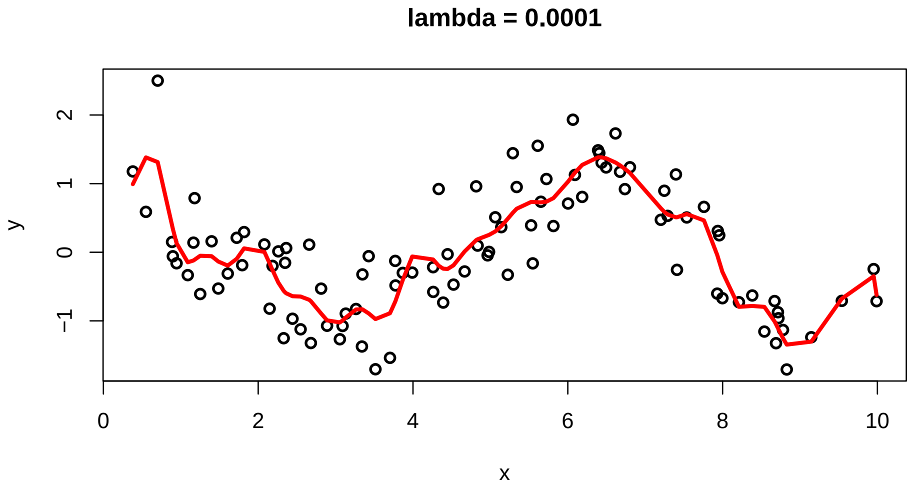
Example (KRR with Gaussian RBF kernel)



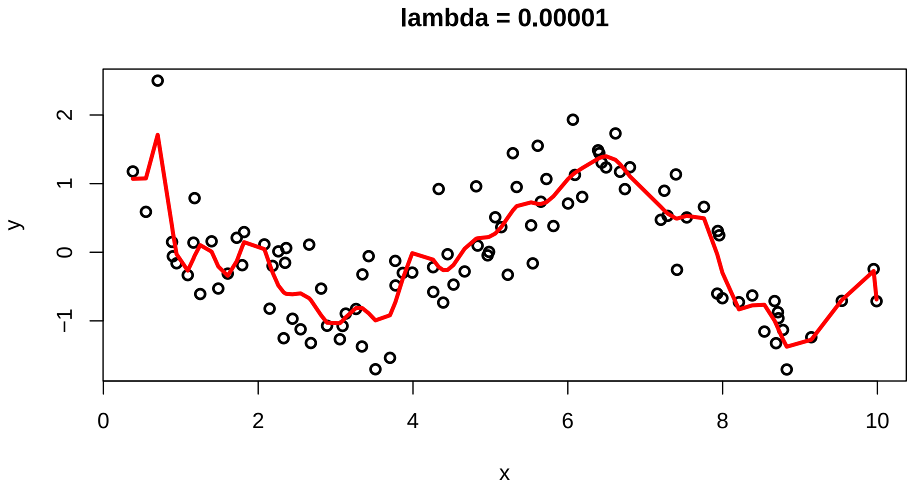
Example (KRR with Gaussian RBF kernel)



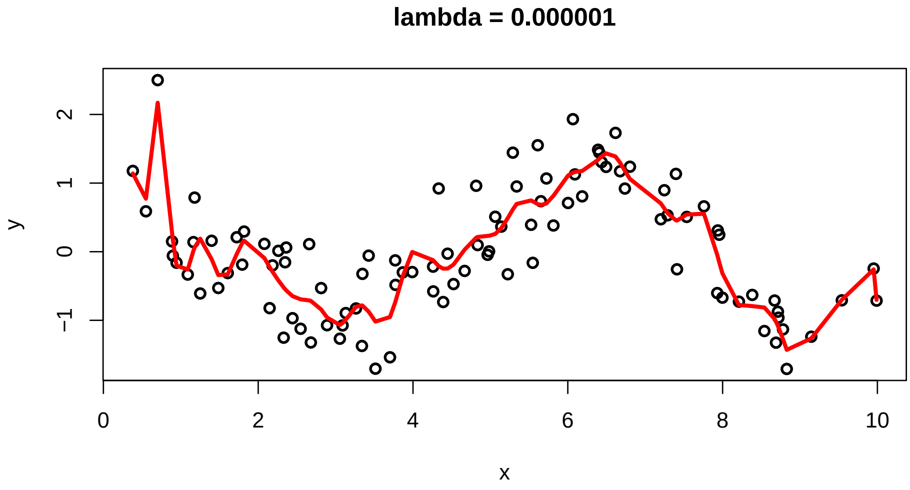
Example (KRR with Gaussian RBF kernel)



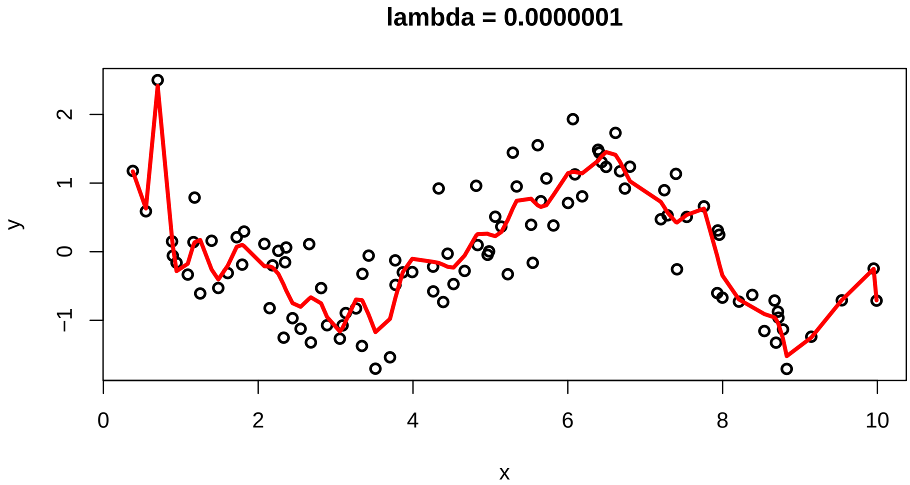
Example (KRR with Gaussian RBF kernel)



Example (KRR with Gaussian RBF kernel)



Example (KRR with Gaussian RBF kernel)



Remark: uniqueness of the solution

Let us find *all* α's that solve

$$K\left[\left(K+\lambda n I\right)\alpha - Y\right] = 0$$

- K being a symmetric matrix, it can be diagonalized in an orthonormal basis and $Ker(K) \perp Im(K)$.
- In this basis we see that $\left(K+\lambda n I\right)^{-1}$ leaves $Im(K)$ and $Ker(K)$ invariant.
- The problem is therefore equivalent to:

$$\begin{aligned} &\left(K+\lambda n I\right)\alpha - Y \in Ker(K) \\ \Leftrightarrow &\alpha - \left(K+\lambda n I\right)^{-1} Y \in Ker(K) \\ \Leftrightarrow &\alpha = \left(K+\lambda n I\right)^{-1} Y + \epsilon, \text{ with } K\epsilon = 0. \end{aligned}$$

- However, if $\alpha' = \alpha + \epsilon$ with $K\epsilon = 0$, then:

$$\| \beta - \beta' \|_2^2 = \left(\alpha - \alpha'\right)^\top K \left(\alpha - \alpha'\right) = 0\,,$$

  therefore $\beta = \beta'$. KRR has a unique solution β, which can possibly be expressed by several α's if K is singular.

Comparison with "standard" ridge regression

- Let X the $n \times p$ data matrix, $K = XX^\top$ the kernel Gram matrix.
- In "standard" ridge regression, we have $\hat{f}(x) = \hat{\beta}^\top x$ with

$$\hat{\beta} = \left(X^\top X + n\lambda I\right)^{-1} X^\top Y \,.$$

- In "kernel" ridge regression, we have $\tilde{f}(x) = \sum_{i=1}^n \alpha_i x_i^\top x = \tilde{\beta}^\top x$ with

$$\tilde{\beta} = \sum_{i=1}^n \alpha_i x_i = X^\top \alpha = X^\top \left(XX^\top + \lambda n I\right)^{-1} Y \,.$$

- Oups... which one is correct?

Comparison with "standard" ridge regression

Matrix inversion lemma

For any matrices B and C, and $\gamma > 0$ the following holds (when it makes sense):

$$B\left(CB + \gamma I\right)^{-1} = \left(BC + \gamma I\right)^{-1} B$$

We deduce that (of course...):

$$\hat{\beta} = \underbrace{\left(X^\top X + n\lambda I\right)^{-1}}_{p\times p} X^\top Y = X^\top \underbrace{\left(XX^\top + \lambda n I\right)^{-1}}_{n\times n} Y = \tilde{\beta}$$

Computationally, inverting the matrix is the expensive part, which suggest to implement:

- KRR when $p > n$ (high dimension)
- RR when $p < n$ (many points)

Generalization

- We learn the function $f(x) = \sum_{i=1}^{n} \alpha_i K(x_i, x)$ by solving in α the following optimization problem, with adequate loss function ℓ:

$$\min_{\alpha \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^{n} \ell \left(\sum_{j=1}^{n} \alpha_j K(x_i, x_j), y_i \right) + \lambda \sum_{i,j=1}^{n} \alpha_i \alpha_j K(x_i, x_j) \,.$$

- No explicit solution, but convex optimization problem
- Note that the dimension of the problem is now n instead of p (useful when $n < p$)

The case of SVM

- Soft-margin SVM with a kernel solves:

$$\min_{\alpha\in\mathbb{R}^n, b\in\mathbb{R}} \left\{ \sum_{i=1}^n \ell_{\text{hinge}}\left(\sum_{j=1}^n \alpha_j K(x_i, x_j), y_i \right) + \lambda \sum_{i,j=1}^n \alpha_i \alpha_j K(x_i, x_j) \right\} .$$

- By Lagrange duality we saw that this is equivalent to

$$\max_{\alpha\in\mathbb{R}^n} L(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2}\sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j K(x_i, x_j) + b\,,$$

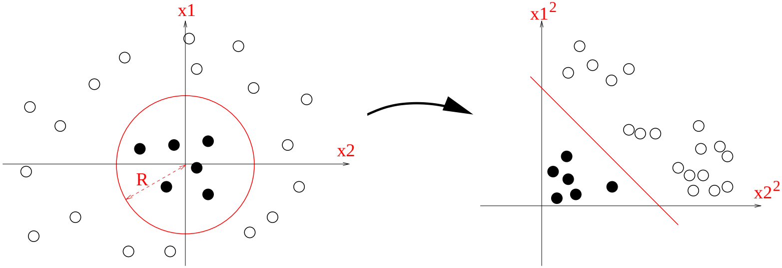
under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C, & \text{for } i = 1, \ldots, n \\ \sum_{i=1}^n \alpha_i y_i = 0\,. \end{cases}$$

- This is not a surprise, both problems are also dual to each other (*exercise*).

Outline

Remember: polynomial kernel



$$\forall x, x' \in \mathbb{R}^p, \qquad K(x, x') = \left(x^\top x' + 1\right)^d$$

is an inner product in a feature space of all monomials of degree up to d

Which functions $K(x, x')$ are kernels?

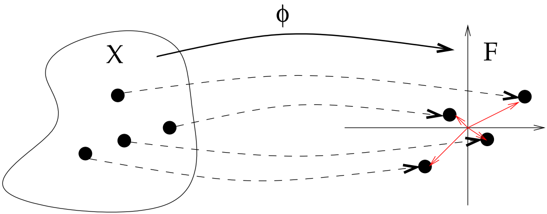
Definition

A function $K(x, x')$ defined on a set $\mathcal{X}$ is a kernel if and only if there exists a features space (Hilbert space) $\mathcal{H}$ and a mapping

$$\Phi : \mathcal{X} \mapsto \mathcal{H} \,,$$

such that, for any x, x' in $\mathcal{X}$:

$$K\left(x, x'\right) = \left\langle \Phi\left(x\right), \Phi\left(x'\right)\right\rangle_{\mathcal{H}} \,.$$



Reminder ...

- An inner product on an $\mathbb{R}$-vector space $\mathcal{H}$ is a mapping $(f, g) \mapsto \langle f, g \rangle_{\mathcal{H}}$ from $\mathcal{H}^2$ to $\mathbb{R}$ that is bilinear, symmetric and such that $\langle f, f \rangle > 0$ for all $f \in \mathcal{H} \backslash \{0\}$.
- A vector space endowed with an inner product is called pre-Hilbert. It is endowed with a norm defined by the inner product as $\| f \|_{\mathcal{H}} = \langle f, f \rangle_{\mathcal{H}}^{\frac{1}{2}}$.
- A Hilbert space is a pre-Hilbert space complete for the norm defined by the inner product.

Kernel examples

- Polynomial (on $\mathbb{R}^d$):

$$K(x, x') = (x.x' + 1)^d$$

- Gaussian radial basis function (RBF) (on $\mathbb{R}^d$)

$$K(x, x') = \exp\left(-\frac{||x - x'||^2}{2\sigma^2}\right)$$

- Laplace kernel (on $\mathbb{R}$)

$$K(x, x') = \exp\left(-\gamma|x - x'|\right)$$

- Min kernel (on $\mathbb{R}_+$)

$$K(x, x') = \min(x, x')$$

Example: SVM with a Gaussian kernel

- Training:

$$\min_{\alpha \in \mathbb{R}^n} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \exp\left(-\frac{||\vec{x}_i - \vec{x}_j||^2}{2\sigma^2}\right)$$

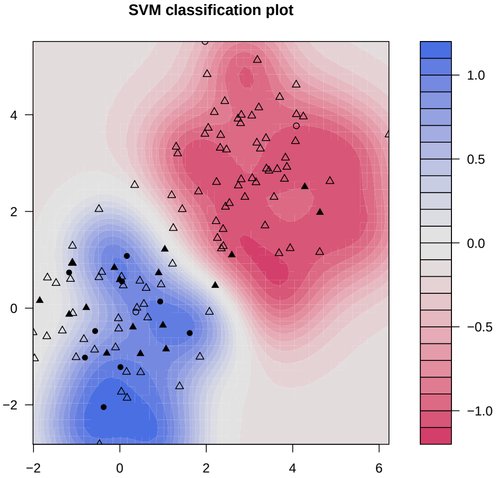
$$\text{s.t. } 0 \leq \alpha_i \leq C, \quad \text{and } \sum_{i=1}^{n} \alpha_i y_i = 0.$$

- Prediction

$$f(\vec{x}) = \sum_{i=1}^{n} \alpha_i \exp\left(-\frac{||\vec{x} - \vec{x}_i||^2}{2\sigma^2}\right)$$

Example: SVM with a Gaussian kernel

$$f(\vec{x}) = \sum_{i=1}^{n} \alpha_i \exp\left(-\frac{||\vec{x} - \vec{x}_i||^2}{2\sigma^2}\right)$$



Positive Definite (p.d.) functions

Definition

A positive definite (p.d.) function on the set $\mathcal{X}$ is a function $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ symmetric:

$$\forall \left(x, x'\right) \in \mathcal{X}^2, \quad K\left(x, x'\right) = K\left(x', x\right),$$

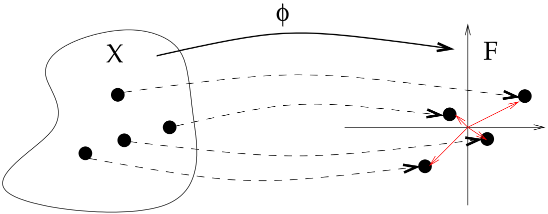
and which satisfies, for all $N \in \mathbb{N}$, $(x_1, x_2, \ldots, x_N) \in \mathcal{X}^N$ et $(a_1, a_2, \ldots, a_N) \in \mathbb{R}^N$:

$$\sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j K\left(x_i, x_j\right) \geq 0.$$

Kernels are p.d. functions

Theorem (Aronszajn, 1950)

K is a kernel if and only if it is a positive definite function.



Proof: kernel $\implies$ p.d. (easy)

Let

$$K(x, x') = \left\langle \Phi(x), \Phi(x') \right\rangle_{\mathcal{H}}$$

be a kernel. It is p.d. because:

- $K(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}} = \langle \Phi(x'), \Phi(x) \rangle_{\mathcal{H}} = K(x', x)$,
- $\sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j \langle \Phi(x_i), \Phi(x_j) \rangle_{\mathcal{H}} = \| \sum_{i=1}^{N} a_i \Phi(x_i) \|_{\mathcal{H}}^2 \geq 0$.

Proof: p.d. $\implies$ kernel when $\mathcal{X}$ is finite

- Suppose $\mathcal{X} = \{x_1, x_2, \ldots, x_N\}$ is finite of size N.
- Any p.d. kernel $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is entirely defined by the $N \times N$ symmetric positive semidefinite matrix $[K]_{ij} := K(x_i, x_j)$.
- It can therefore be diagonalized on an orthonormal basis of eigenvectors $(u_1, u_2, \ldots, u_N)$, with non-negative eigenvalues $0 \leq \lambda_1 \leq \ldots \leq \lambda_N$, i.e.,

$$K(x_i, x_j) = \left[\sum_{l=1}^{N} \lambda_l u_l u_l^\top\right]_{ij} = \sum_{l=1}^{N} \lambda_l u_l(i) u_l(j) = \langle \Phi(x_i), \Phi(x_j) \rangle_{\mathbb{R}^N},$$

with

$$\Phi(x_i) = \begin{pmatrix} \sqrt{\lambda_1} u_1(i) \\ \vdots \\ \sqrt{\lambda_N} u_N(i) \end{pmatrix}. \qquad \square$$

Proof: p.d. $\Longrightarrow$ kernel in the general case

- Mercer (1909) for $\mathcal{X} = [a, b] \subset \mathbb{R}$ (more generally $\mathcal{X}$ compact) and K continuous (the so-called Mercer kernels).
- Kolmogorov (1941) for $\mathcal{X}$ countable.
- Aronszajn (1944, 1950) for the general case, using the theory of RKHS.

Definition

Let $\mathcal{X}$ be a set and $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$ be a class of functions forming a (real) Hilbert space with inner product $\langle .,. \rangle_{\mathcal{H}}$. The function $K : \mathcal{X}^2 \mapsto \mathbb{R}$ is called a reproducing kernel (r.k.) of $\mathcal{H}$ if

1. $\mathcal{H}$ contains all functions of the form

$$\forall x \in \mathcal{X}, \quad K_x : t \mapsto K(x,t) \ .$$

2. For every $x \in \mathcal{X}$ and $f \in \mathcal{H}$ the reproducing property holds:

$$f(x) = \langle f, K_x \rangle_{\mathcal{H}} \ .$$

If a r.k. exists, then $\mathcal{H}$ is called a reproducing kernel Hilbert space (RKHS).

An equivalent definition of RKHS

Theorem

The Hilbert space $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$ is a RKHS if and only if for any $x \in \mathcal{X}$, the mapping:

$$\begin{aligned} F : \quad \mathcal{H} &\to \mathbb{R} \\ f &\mapsto f(x) \end{aligned}$$

is continuous.

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is continuous.

Corollary

Convergence in a RKHS implies pointwise convergence, i.e., if $(f_n)_{n\in\mathbb{N}}$ converges to f in $\mathcal{H}$, then $(f_n(x))_{n\in\mathbb{N}}$ converges to $f(x)$ for any $x \in \mathcal{X}$.

Proof

If $\mathcal{H}$ is a RKHS then $f \mapsto f(x)$ is continuous

If a r.k. K exists, then for any $(x, f) \in \mathcal{X} \times \mathcal{H}$:

$$\begin{aligned} |f(x)| &= |\langle f, K_x \rangle_{\mathcal{H}}| \\ &\leq \| f \|_{\mathcal{H}} . \| K_x \|_{\mathcal{H}} \text{ (Cauchy-Schwarz)} \\ &\leq \| f \|_{\mathcal{H}} . K(x, x)^{\frac{1}{2}} \ , \end{aligned}$$

because $\| K_x \|_{\mathcal{H}}^2 = \langle K_x, K_x \rangle_{\mathcal{H}} = K(x, x)$. Therefore $f \in \mathcal{H} \mapsto f(x) \in \mathbb{R}$ is a continuous linear mapping. $\square$

Proof (Converse)

If $f \mapsto f(x)$ is continuous then $\mathcal{H}$ is a RKHS

Conversely, let us assume that for any $x \in \mathcal{X}$ the linear form $f \in \mathcal{H} \mapsto f(x)$ is continuous.
Then by Riesz representation theorem there (general property of Hilbert spaces) there exists a unique $g_x \in \mathcal{H}$ such that:

$$f(x) = \langle f, g_x \rangle_{\mathcal{H}}$$

The function $K(x, y) = g_x(y)$ is then a r.k. for $\mathcal{H}$. $\square$

Unicity of r.k. and RKHS

Theorem

- If $\mathcal{H}$ is a RKHS, then it has a unique r.k.
- Conversely, a function K can be the r.k. of at most one RKHS.

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- Conversely, a function K can be the r.k. of at most one RKHS.

Consequence

This shows that we can talk of "the" kernel of a RKHS, or "the" RKHS of a kernel.

Proof

If a r.k. exists then it is unique

Let K and K' be two r.k. of a RKHS $\mathcal{H}$. Then for any $x \in \mathcal{X}$:

$$\begin{aligned}
\| K_x - K'_x \|^2_{\mathcal{H}} &= \langle K_x - K'_x, K_x - K'_x \rangle_{\mathcal{H}} \\
&= \langle K_x - K'_x, K_x \rangle_{\mathcal{H}} - \langle K_x - K'_x, K'_x \rangle_{\mathcal{H}} \\
&= K_x(x) - K'_x(x) - K_x(x) + K'_x(x) \\
&= 0 \,.
\end{aligned}$$

This shows that $K_x = K'_x$ as functions, i.e., $K_x(y) = K'_x(y)$ for any $y \in \mathcal{X}$. In other words, K=K'. $\square$

Proof

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The RKHS of a r.k. K is unique

Left as exercice.

An important result

Theorem

A function $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is p.d. if and only if it is a r.k.

Proof: r.k. $\implies$ p.d.

1. A r.k. is symmetric because, for any $(x, y) \in \mathcal{X}^2$:

$$K(x, y) = \langle K_x, K_y \rangle_{\mathcal{H}} = \langle K_y, K_x \rangle_{\mathcal{H}} = K(y, x) .$$

2. It is p.d. because for any $N \in \mathbb{N}$,$(x_1, x_2, \ldots, x_N) \in \mathcal{X}^N$, and $(a_1, a_2, \ldots, a_N) \in \mathbb{R}^N$:

$$\begin{aligned}\sum_{i,j=1}^{N} a_i a_j K(x_i, x_j) &= \sum_{i,j=1}^{N} a_i a_j \left\langle K_{x_i}, K_{x_j} \right\rangle_{\mathcal{H}} \\ &= \| \sum_{i=1}^{N} a_i K_{x_i} \|_{\mathcal{H}}^2 \\ &\geq 0. \quad \square\end{aligned}$$

- Let $\mathcal{H}_0$ be the vector subspace of $\mathbb{R}^{\mathcal{X}}$ spanned by the functions $\{K_x\}_{x\in\mathcal{X}}$.
- For any $f, g \in \mathcal{H}_0$, given by:

$$f = \sum_{i=1}^{m} a_i K_{x_i}, \quad g = \sum_{j=1}^{n} b_j K_{y_j},$$

let:

$$\langle f, g \rangle_{\mathcal{H}_0} := \sum_{i,j} a_i b_j K\left(x_i, y_j\right).$$

Proof: p.d. $\implies$ r.k. (2/4)

- $\langle f, g \rangle_{\mathcal{H}_0}$ does not depend on the expansion of f and g because:

$$\langle f, g \rangle_{\mathcal{H}_0} = \sum_{i=1}^{m} a_i g\left(x_i\right) = \sum_{j=1}^{n} b_j f\left(y_j\right).$$

- This also shows that $\langle ., . \rangle_{\mathcal{H}_0}$ is a symmetric bilinear form.
- This also shows that for any $x \in \mathcal{X}$ and $f \in \mathcal{H}_0$:

$$\langle f, K_x \rangle_{\mathcal{H}_0} = f\left(x\right).$$

- K is assumed to be p.d., therefore:

$$\| f \|_{\mathcal{H}_0}^2 = \sum_{i,j=1}^{m} a_i a_j K(x_i, x_j) \geq 0 \, .$$

  In particular Cauchy-Schwarz is valid with $\langle .,. \rangle_{\mathcal{H}_0}$.

- By Cauchy-Schwarz we deduce that $\forall x \in \mathcal{X}$:

$$| f(x) | = \left| \langle f, K_x \rangle_{\mathcal{H}_0} \right| \leq \| f \|_{\mathcal{H}_0} . K(x,x)^{\frac{1}{2}} \, ,$$

  therefore $\| f \|_{\mathcal{H}_0} = 0 \implies f = 0$.

- $\mathcal{H}_0$ is therefore a pre-Hilbert space endowed with the inner product $\langle .,. \rangle_{\mathcal{H}_0}$.

- For any Cauchy sequence $(f_n)_{n\geq 0}$ in $\left(\mathcal{H}_0, \langle ., . \rangle_{\mathcal{H}_0}\right)$, we note that:

  $$\forall (x, m, n) \in \mathcal{X} \times \mathbb{N}^2, \quad | f_m(x) - f_n(x) | \leq \| f_m - f_n \|_{\mathcal{H}_0} . K(x, x)^{\frac{1}{2}} .$$

  Therefore for any x the sequence $(f_n(x))_{n\geq 0}$ is Cauchy in $\mathbb{R}$ and has therefore a limit.
- If we add to $\mathcal{H}_0$ the functions defined as the pointwise limits of Cauchy sequences, then the space becomes complete and is therefore a Hilbert space, with K as r.k. (up to a few technicalities, left as exercice). $\square$

Application: back to Aronszajn's theorem

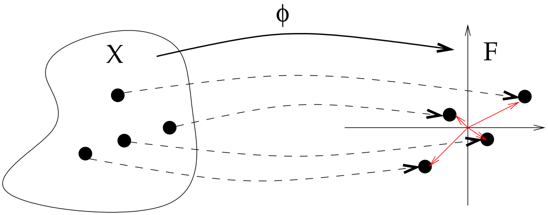
Theorem (Aronszajn, 1950)

K is a p.d. kernel on the set $\mathcal{X}$ if and only if there exists a Hilbert space $\mathcal{H}$ and a mapping

$$\Phi : \mathcal{X} \mapsto \mathcal{H} \,,$$

such that, for any x, x' in $\mathcal{X}$:

$$K\left(x, x'\right) = \left\langle \Phi\left(x\right), \Phi\left(x'\right) \right\rangle_{\mathcal{H}} \,.$$



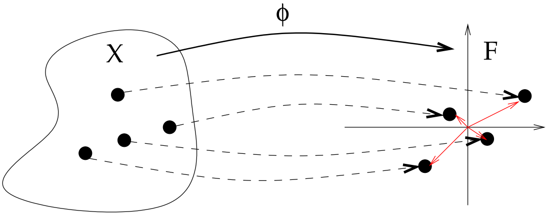
Proof of Aronzsajn's theorem: p.d. $\implies$ kernel

- If K is p.d. over a set $\mathcal{X}$ then it is the r.k. of a Hilbert space $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$.
- Let the mapping $\Phi : \mathcal{X} \to \mathcal{H}$ defined by:

$$\forall x \in \mathcal{X}\,, \quad \Phi(x) = K_x\,.$$

- By the reproducing property we have:

$$\forall (x, y) \in \mathcal{X}^2, \quad \langle \Phi(x), \Phi(y) \rangle_{\mathcal{H}} = \langle K_x, K_y \rangle_{\mathcal{H}} = K(x, y)\,. \qquad \square$$



RKHS of the linear kernel

- Let $\mathcal{X} = \mathbb{R}^d$ and $K(x, y) = \langle x, y \rangle_{\mathbb{R}^d}$ be the linear kernel
- The corresponding RKHS consists of functions:

$$x \in \mathbb{R}^d \mapsto f(x) = \sum_i a_i \langle x_i, x \rangle_{\mathbb{R}^d} = \langle w, x \rangle_{\mathbb{R}^d} \ ,$$

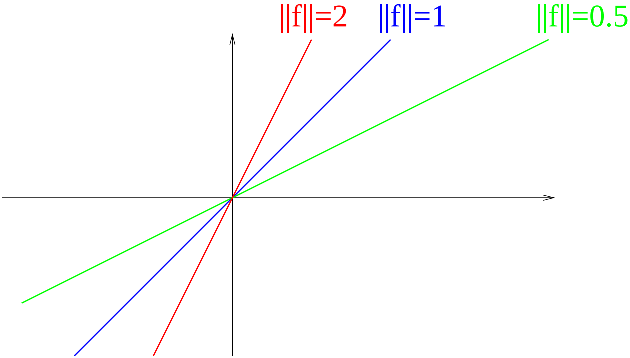
  with $w = \sum_i a_i x_i$.
- The RKHS is therefore the set of linear forms endowed with the following inner product:

$$\langle f, g \rangle_{\mathcal{H}_K} = \langle w, v \rangle_{\mathbb{R}^d} \ ,$$

  when $f(x) = w^\top x$ and $g(x) = v^\top x$.

RKHS of the linear kernel (cont.)

$$\begin{cases} K_{lin}(x, x') & = x^\top x' \ . \\ f(x) & = w^\top x \ , \\ \| f \|_{\mathcal{H}} & = \| w \|_2 \ . \end{cases}$$



$$f_\beta(x) = \beta^\top \Phi(x)\,, \quad \min_{\beta \in \mathbb{R}^p} \left\{ \frac{1}{n} \sum_{i=1}^{n} \ell(f_\beta(x_i), y_i) + \lambda \|\beta\|_2^2 \right\}$$

is equivalent to

$$\min_{f \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) + \lambda \|f\|_{\mathcal{H}}^2 \right\}$$

where $\mathcal{H}$ is the RKHS of the kernel $K(x, x') = \Phi(x)^\top \Phi(x')$.

Smoothness functional

A simple inequality

- By Cauchy-Schwarz we have, for any function $f \in \mathcal{H}$ and any two points $x, x' \in \mathcal{X}$:

$$
\begin{aligned}
\left| f(x) - f\left(x'\right) \right| &= \left| \langle f, K_x - K_{x'} \rangle_{\mathcal{H}} \right| \\
&\leq \| f \|_{\mathcal{H}} \times \| K_x - K_{x'} \|_{\mathcal{H}} \\
&= \| f \|_{\mathcal{H}} \times d_K\left(x, x'\right) .
\end{aligned}
$$

- The norm of a function in the RKHS controls how fast the function varies over $\mathcal{X}$ with respect to the geometry defined by the kernel (Lipschitz with constant $\| f \|_{\mathcal{H}}$).

Important message

$$\text{Small norm} \implies \text{slow variations.}$$

Kernels and RKHS : Summary

- P.d. kernels can be thought of as inner product after embedding the data space $\mathcal{X}$ in some Hilbert space. As such a p.d. kernel defines a metric on $\mathcal{X}$.
- A realization of this embedding is the RKHS, valid without restriction on the space $\mathcal{X}$ nor on the kernel.
- The RKHS is a space of functions over $\mathcal{X}$. The norm of a function in the RKHS is related to its degree of smoothness w.r.t. the metric defined by the kernel on $\mathcal{X}$.
- ℓ_2-regularized learning in the feature space can be formulated in the RKHS

$$\min_{f \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) + \lambda \|f\|_{\mathcal{H}}^2 \right\}$$

Outline

Kernel examples

- Polynomial (on $\mathbb{R}^d$):

$$K(x,x') = (x.x' + 1)^d$$

- Gaussian radial basis function (RBF) (on $\mathbb{R}^d$)

$$K(x,x') = \exp\left(-\frac{||x-x'||^2}{2\sigma^2}\right)$$

- Laplace kernel (on $\mathbb{R}$)

$$K(x,x') = \exp\left(-\gamma|x-x'|\right)$$

- Min kernel (on $\mathbb{R}_+$)

$$K(x,x') = \min(x,x')$$

Exercice

Exercice: for each kernel, find a Hilbert space $\mathcal{H}$ and a mapping $\Phi : \mathcal{X} \to \mathcal{H}$ such that $K(x,x') = \langle\Phi(x), \Phi(x')\rangle$

Example: SVM with a Gaussian kernel

- Training:

$$\min_{\alpha \in \mathbb{R}^n} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \exp\left(-\frac{||\vec{x}_i - \vec{x}_j||^2}{2\sigma^2}\right)$$

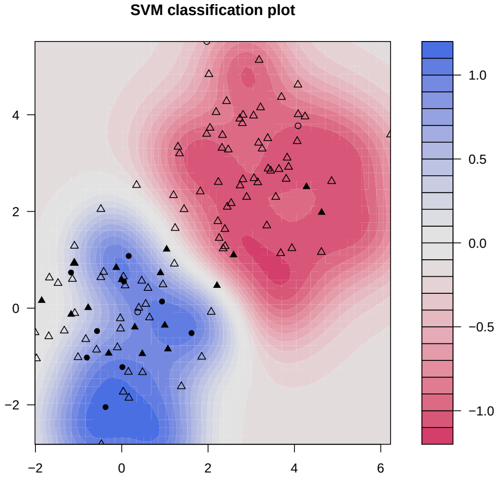
$$\text{s.t. } 0 \leq \alpha_i \leq C, \quad \text{and } \sum_{i=1}^{n} \alpha_i y_i = 0.$$

- Prediction

$$f(\vec{x}) = \sum_{i=1}^{n} \alpha_i \exp\left(-\frac{||\vec{x} - \vec{x}_i||^2}{2\sigma^2}\right)$$

Example: SVM with a Gaussian kernel

$$f(\vec{x}) = \sum_{i=1}^{n} \alpha_i \exp\left(-\frac{||\vec{x} - \vec{x}_i||^2}{2\sigma^2}\right)$$



How to choose or make a kernel?

- Design features
- Design a distance or similarity measure
- Design a regularizer on f

Example: Sobolev norm as regularizer

Theorem

Let $\mathcal{X} = [0,1]$ and the kernel:

$$\forall (x,y) \in [0,1]^2, \quad K(x,y) = \min(x,y).$$

Then the RKHS is

$$\mathcal{H} = \left\{ f : [0,1] \mapsto \mathbb{R}, \text{absolutely continuous}, f' \in L^2([0,1]), f(0) = 0 \right\}.$$

and the regularizer is a Sobolev norm

$$\Omega(f) = \| f \|_{\mathcal{H}}^2 = \int_0^1 f'(u)^2 \, du = \| f' \|_{L^2([0,1])}^2.$$

Proof (1/5)

Sketch

We need to show that

- $\mathcal{H}$ is a Hilbert space
- $\forall x \in [0, 1]$, $K_x \in \mathcal{H}$,
- $\forall (x, f) \in [0, 1] \times \mathcal{H}, \langle f, K_x \rangle_{\mathcal{H}} = f(x)$.

Proof (2/5)

$\mathcal{H}$ is a pre-Hilbert space

- f absolutely continuous implies differentiable almost everywhere, and

$$\forall x \in [0,1], \quad f(x) = f(0) + \int_0^x f'(u)du\,.$$

- For any $f \in \mathcal{H}$, $f(0) = 0$ implies by Cauchy-Schwarz:

$$|\, f\,(x)\,| = \left| \int_0^x f'(u)du \right| \leq \sqrt{x} \left(\int_0^1 f'(u)^2 du \right)^{\frac{1}{2}} = \sqrt{x} \|\, f\,\|_{\mathcal{H}}\,.$$

Therefore, $\|\, f\,\|_{\mathcal{H}} = 0 \implies f = 0$, showing that $\langle .,. \rangle_{\mathcal{H}}$ is an inner product. $\mathcal{H}$ is thus a pre-Hilbert space.

Proof (3/5)

$\mathcal{H}$ is a Hilbert space

- To show that $\mathcal{H}$ is complete, let $(f_n)_{n\in\mathbb{N}}$ a Cauchy sequence in $\mathcal{H}$
- $(f_n')_{n\in\mathbb{N}}$ is a Cauchy sequence in $L^2[0,1]$, thus converges to $g \in L^2[0,1]$
- By the previous inequality, $(f_n(x))_{n\in\mathbb{N}}$ is a Cauchy sequence and thus converges to a real number $f(x)$, for any $x \in [0,1]$. Moreover:

$$f(x) = \lim_n f_n(x) = \lim_n \int_0^x f_n'(u)du = \int_0^x g(u)du\,,$$

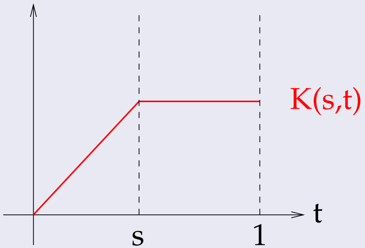
  showing that f is absolutely continuous and $f' = g$ almost everywhere; in particular, $f' \in L^2[0,1]$.
- Finally, $f(0) = \lim_n f_n(0) = 0$, therefore $f \in \mathcal{H}$ and

$$\lim_n \| f_n - f \|_{\mathcal{H}} = \| f' - g_n \|_{L^2[0,1]} = 0\,.$$

Proof (4/5)

$\forall x \in [0,1]$, $K_x \in \mathcal{H}$

Let $K_x(y) = K(x,y) = \min(x,y)$ sur $[0,1]^2$:



K_x is differentiable except at s, has a square integrable derivative, and $K_x(0) = 0$, therefore $K_x \in \mathcal{H}$ for all $x \in [0,1]$. $\square$

Proof (5/5)

For all x, f, $\langle f, K_x \rangle_{\mathcal{H}} = f(x)$

For any $x \in [0, 1]$ and $f \in \mathcal{H}$ we have:

$$\langle f, K_x \rangle_{\mathcal{H}} = \int_0^1 f'(u) K_x'(u) du = \int_0^x f'(u) du = f(x),$$

which shows that K is the r.k. associated to $\mathcal{H}$. $\square$

Theorem

Let $\mathcal{X} = \mathbb{R}^d$ and D a differential operator on a class of functions $\mathcal{H}$ such that, endowed with the inner product:

$$\forall (f, g) \in \mathcal{H}^2, \quad \langle f, g \rangle_{\mathcal{H}} = \langle Df, Dg \rangle_{L^2(\mathcal{X})},$$

it is a Hilbert space.
Then $\mathcal{H}$ is a RKHS that admits as r.k. the Green function of the operator D^*D, where D^* denotes the adjoint operator of D.

Green functions

Let the differential equation on $\mathcal{H}$:

$$f = Dg \, ,$$

where g is unknown. In order to solve it we can look for g of the form:

$$g\left(x\right) = \int_{\mathcal{X}} k\left(x, y\right) f\left(y\right) dy$$

for some function $k : \mathcal{X}^2 \mapsto \mathbb{R}$. k must then satisfy, for all $x \in \mathcal{X}$,

$$f\left(x\right) = Dg\left(x\right) = \left\langle Dk_x, f \right\rangle_{L^2(\mathcal{X})} \, .$$

k is called the Green function of the operator D.

Proof

Let $\mathcal{H}$ be a Hilbert space endowed with the inner product:

$$\langle f, g \rangle_{\mathcal{X}} = \langle Df, Dg \rangle_{L^2(\mathcal{X})} ,$$

and K be the Green function of the operator $D^* D$. For all $x \in \mathcal{X}$, $K_x \in \mathcal{H}$ because:

$$\langle DK_x, DK_x \rangle_{L^2(\mathcal{X})} = \langle D^* DK_x, K_x \rangle_{L^2(\mathcal{X})} = K_x(x) < \infty .$$

Moreover, for all $f \in \mathcal{H}$ and $x \in \mathcal{X}$, we have:

$$f(x) = \langle D^* DK_x, f \rangle_{L^2(\mathcal{X})} = \langle DK_x, Df \rangle_{L^2(\mathcal{X})} = \langle K_x, f \rangle_{\mathcal{H}} ,$$

which shows that $\mathcal{H}$ is a RKHS with K as r.k. $\square$

Translation invariant kernels

Definition

A kernel $K : \mathbb{R}^d \times \mathbb{R}^d \mapsto \mathbb{R}$ is called translation invariant (t.i.) if it only depends on the difference between its argument, i.e.:

$$\forall (x, y) \in \mathbb{R}^{2d}, \quad K(x, y) = \kappa(x - y).$$

Theorem (Bochner)

A real-valued function $\kappa(x - y)$ on $\mathbb{R}^d$ is positive definite if and only if it is the Fourier transform of a symmetric, positive, and finite Borel measure.

RKHS of translation invariant kernels

Theorem

Let K be a translation invariant p.d. kernel, such that κ is integrable on $\mathbb{R}^d$ as well as its Fourier transform $\hat{\kappa}$. The subset $\mathcal{H}_K$ of $L_2\left(\mathbb{R}^d\right)$ that consists of integrable and continuous functions f such that:

$$\| f \|_K^2 := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{\left| \hat{f}(\omega) \right|^2}{\hat{\kappa}(\omega)} d\omega < +\infty \,,$$

endowed with the inner product:

$$\langle f, g \rangle := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{\hat{f}(\omega) \hat{g}(\omega)^*}{\hat{\kappa}(\omega)} d\omega$$

is a RKHS with K as r.k.

Example: Gaussian RBF kernel

$$K(x,y) = e^{-\frac{(x-y)^2}{2\sigma^2}}$$

corresponds to:

$$\hat{\kappa}(\omega) = e^{-\frac{\sigma^2\omega^2}{2}}$$

and

$$\| f \|_{\mathcal{H}}^2 = \int \left| \hat{f}(\omega) \right|^2 e^{\frac{\sigma^2\omega^2}{2}} d\omega \,.$$

In particular, all functions in $\mathcal{H}$ are infinitely differentiable with all derivatives in L^2.

Example: Laplace kernel

$$K(x,y) = \frac{1}{2} e^{-\gamma | x-y |}$$

corresponds to:

$$\hat{\kappa}(\omega) = \frac{\gamma}{\gamma^2 + \omega^2}$$

and

$$\| f \|_{\mathcal{H}}^2 = \int \left| \hat{f}(\omega) \right|^2 \frac{\left(\gamma^2 + \omega^2\right)}{\gamma} d\omega \,.$$

The RKHS is the set of functions L^2 differentiable with derivatives in L^2 (Sobolev space).

Example: sinc kernel

$$K(x,y) = \frac{\sin(\Omega(x-y))}{\pi(x-y)}$$

corresponds to:

$$\hat{\kappa}(\omega) = \mathbf{1}(-\Omega \leq \omega \leq \Omega)\,.$$

The RKHS is the set of functions whose spectrum is included in $[-\Omega, \Omega]$:

$$\mathcal{H} = \left\{ f : \int_{|\,\omega\,|>\Omega} \left| \hat{f}(\omega) \right|^2 d\omega = 0 \right\},$$

and

$$\| f \|_{\mathcal{H}}^2 = \int_{|\,\omega\,|\leq\Omega} \left| \hat{f}(\omega) \right|^2 = \int_{\omega\in\mathbb{R}} \left| \hat{f}(\omega) \right|^2 = (2\pi)^d \int_{x\in\mathbb{R}} |\, f(x) \,|^2 \, dx\,.$$

Supervised sequence classification

Data (training)

- Secured proteins:

  MASKATLLLAFTLLFATCIARHQQRQQQNQCQLQNIEA...
  MARSSLFTFLCLAVFINGCLSQIEQQSPWEFQGSEVW...
  MALHTVLIMLSLLPMLEAQNPEHANITIGEPITNETLGWL...
  ...

- Non-secreted proteins:

  MAPPSVFAEVPQAQPVLVFKLIADFREDPDPRKVNLGVG...
  MAHTLGLTQPNSTEPHKISFTAKEIDVIEWKGDILVVG...
  MSISESYAKEIKTAFRQFTDFPIEGEQFEDFLPIIGNP..
  ...

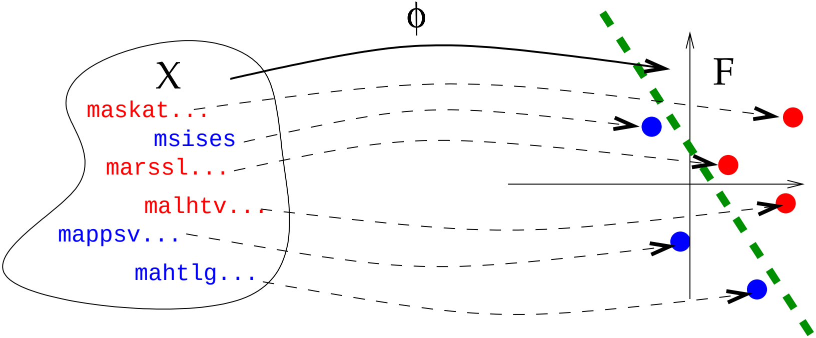
Goal

- Build a classifier to predict whether new proteins are secreted or not.

String kernels

The idea

- Map each string $x \in \mathcal{X}$ to a vector $\Phi(x) \in \mathcal{F}$.
- Train a classifier for vectors on the images $\Phi(x_1), \ldots, \Phi(x_n)$ of the training set (nearest neighbor, linear perceptron, logistic regression, support vector machine...)



Example: substring indexation

The approach

Index the feature space by fixed-length strings, i.e.,

$$\Phi(x) = (\Phi_u(x))_{u \in \mathcal{A}^k}$$

where $\Phi_u(x)$ can be:

- the number of occurrences of u in x (without gaps) : spectrum kernel (Leslie et al., 2002)
- the number of occurrences of u in x up to m mismatches (without gaps) : mismatch kernel (Leslie et al., 2004)
- the number of occurrences of u in x allowing gaps, with a weight decaying exponentially with the number of gaps : substring kernel (Lohdi et al., 2002)

Spectrum kernel (1/2)

Kernel definition

- The 3-spectrum of

$$x = \texttt{CGGSLIAMMWFGV}$$

is:

$$(\texttt{CGG},\texttt{GGS},\texttt{GSL},\texttt{SLI},\texttt{LIA},\texttt{IAM},\texttt{AMM},\texttt{MMW},\texttt{MWF},\texttt{WFG},\texttt{FGV}) \, .$$

- Let $\Phi_u(x)$ denote the number of occurrences of u in x. The k-spectrum kernel is:

$$K(x, x') := \sum_{u \in \mathcal{A}^k} \Phi_u(x) \Phi_u(x') \, .$$

Spectrum kernel (2/2)

Implementation

- The computation of the kernel is formally a sum over $|\mathcal{A}|^k$ terms, but at most $|x| - k + 1$ terms are non-zero in $\Phi(x) \implies$ Computation in $O(|x| + |x'|)$ with pre-indexation of the strings.
- Fast classification of a sequence x in $O(|x|)$:

$$f(x) = w \cdot \Phi(x) = \sum_u w_u \Phi_u(x) = \sum_{i=1}^{|x|-k+1} w_{x_i \dots x_{i+k-1}}.$$

Remarks

- Work with any string (natural language, time series...)
- Fast and scalable, a good default method for string classification.
- Variants allow matching of k-mers up to m mismatches.

Local alignmnent kernel (Saigo et al., 2004)

```
CGGSLIAMM------WFGV
|...|||||....||||
C----LIVMMNRLMWFGV
```

$$
\begin{aligned}
s_{S,g}(\pi) = \; & S(C,C) + S(L,L) + S(I,I) + S(A,V) + 2S(M,M) \\
& + S(W,W) + S(F,F) + S(G,G) + S(V,V) - g(3) - g(4)
\end{aligned}
$$

$$
SW_{S,g}(x,y) := \max_{\pi \in \Pi(x,y)} s_{S,g}(\pi) \quad \text{is not a kernel}
$$

$$
K_{LA}^{(\beta)}(x,y) = \sum_{\pi \in \Pi(x,y)} \exp\left(\beta s_{S,g}(x,y,\pi)\right) \quad \text{is a kernel}
$$

LA kernel is p.d.: proof (1/2)

Definition: Convolution kernel (Haussler, 1999)

Let K_1 and K_2 be two p.d. kernels for strings. The convolution of K_1 and K_2, denoted $K_1 \star K_2$, is defined for any $x, x' \in \mathcal{X}$ by:

$$K_1 \star K_2(x, \mathbf{y}) := \sum_{x_1 x_2 = x, \mathbf{y}_1 \mathbf{y}_2 = \mathbf{y}} K_1(x_1, \mathbf{y}_1) K_2(x_2, \mathbf{y}_2).$$

Lemma

If K_1 and K_2 are p.d. then $K_1 \star K_2$ is p.d..

LA kernel is p.d.: proof (2/2)

$$K_{LA}^{(\beta)} = \sum_{n=0}^{\infty} K_0 \star \left(K_a^{(\beta)} \star K_g^{(\beta)} \right)^{(n-1)} \star K_a^{(\beta)} \star K_0 \,,$$

with

- The constant kernel:

$$K_0\left(x, \mathbf{y}\right) := 1\,.$$

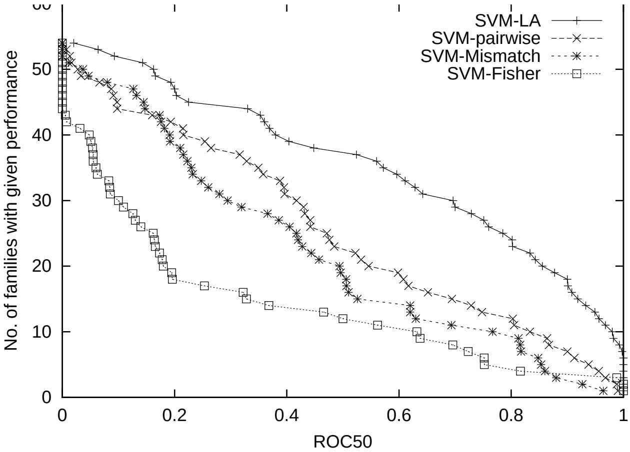
- A kernel for letters:

$$K_a^{(\beta)}\left(x, \mathbf{y}\right) := \begin{cases} 0 & \text{if } \mid x \mid \neq 1 \text{ where } \mid \mathbf{y} \mid \neq 1\,, \\ \exp\left(\beta S(x, \mathbf{y})\right) & \text{otherwise}\,. \end{cases}$$

- A kernel for gaps:

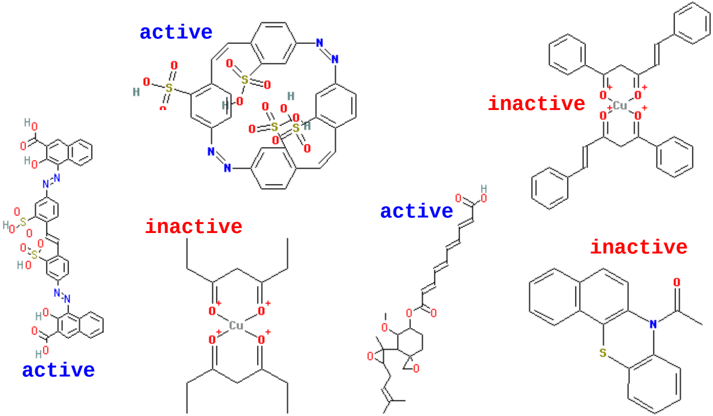
$$K_g^{(\beta)}\left(x, \mathbf{y}\right) = \exp\left[\beta\left(g\left(\mid x \mid\right) + g\left(\mid x \mid\right)\right)\right]\,.$$

The choice of kernel matters



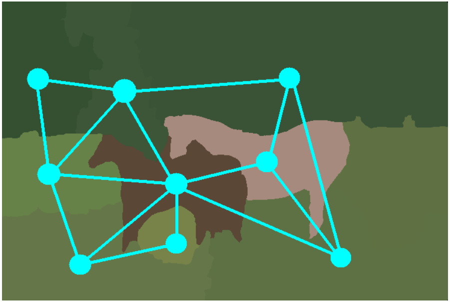
Performance on the SCOP superfamily recognition benchmark (from Saigo et al., 2004).

Virtual screening for drug discovery



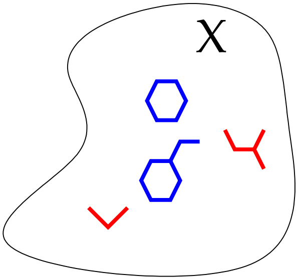
NCI AIDS screen results (from http://cactus.nci.nih.gov).

Image retrieval and classification



From Harchaoui and Bach (2007).

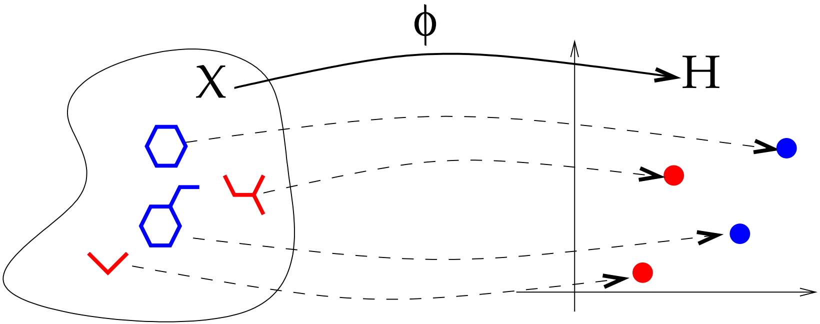
Graph kernels



Graph kernels

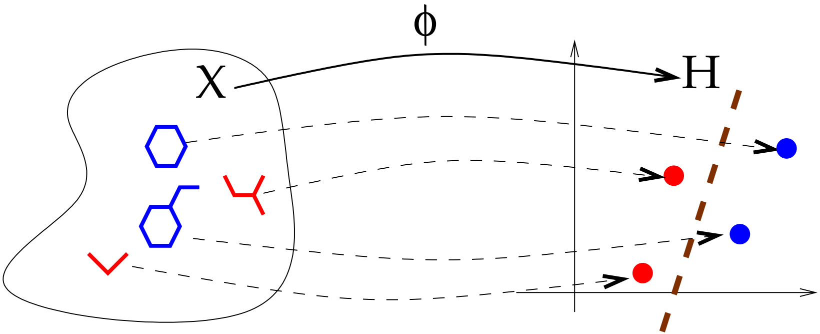
1. Represent each graph x by a vector $\Phi(x) \in \mathcal{H}$, either explicitly or implicitly through the kernel

$$K(x, x') = \Phi(x)^\top \Phi(x') .$$

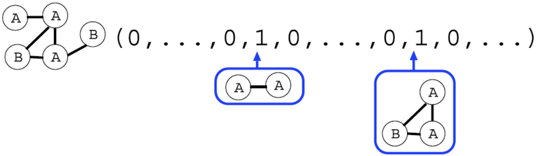


Graph kernels

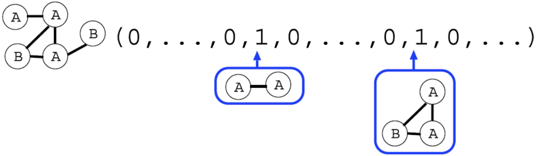
1. Represent each graph x by a vector $\Phi(x) \in \mathcal{H}$, either explicitly or implicitly through the kernel
$$K(x, x') = \Phi(x)^\top \Phi(x') .$$
2. Use a linear method for classification in $\mathcal{H}$.



Indexing by all subgraphs?



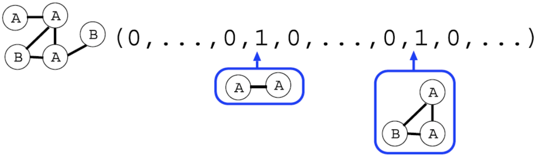
Indexing by all subgraphs?



Theorem

Computing all subgraph occurrences is NP-hard.

Indexing by all subgraphs?



Theorem

Computing all subgraph occurrences is NP-hard.

Proof.

- The linear graph of size n is a subgraph of a graph X with n vertices iff X has an Hamiltonian path
- The decision problem whether a graph has a Hamiltonian path is NP-complete.

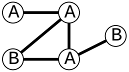
Indexing by specific subgraphs

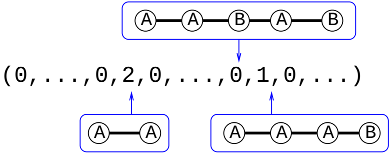
Substructure selection

We can imagine more limited sets of substuctures that lead to more computationnally efficient indexing (non-exhaustive list)

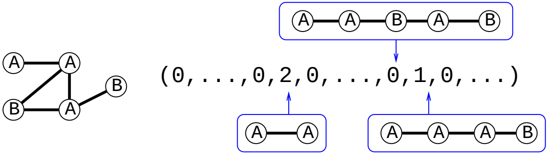
- substructures selected by domain knowledge (MDL fingerprint)
- all path up to length k (Openeye fingerprint, Nicholls 2005)
- all shortest paths (Borgwardt and Kriegel, 2005)
- all subgraphs up to k vertices (graphlet kernel, Sherashidze et al., 2009)
- all frequent subgraphs in the database (Helma et al., 2004)

Example : Indexing by all shortest paths





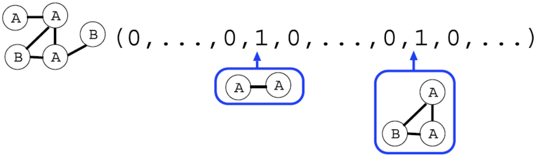
Example : Indexing by all shortest paths



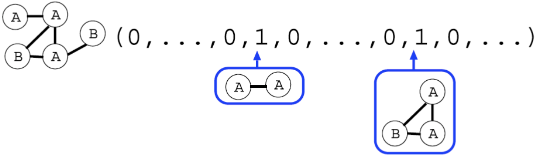
Properties (Borgwardt and Kriegel, 2005)

- There are $O(n^2)$ shortest paths.
- The vector of counts can be computed in $O(n^4)$ with the Floyd-Warshall algorithm.

Example : Indexing by all subgraphs up to k vertices



Example : Indexing by all subgraphs up to k vertices



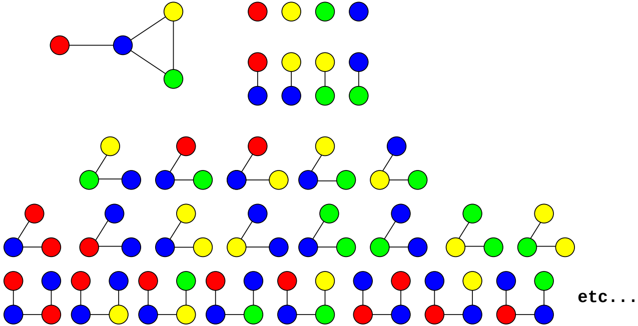
Properties (Shervashidze et al., 2009)

- Naive enumeration scales as $O(n^k)$.
- Enumeration of connected graphlets in $O(nd^{k-1})$ for graphs with degree $\leq d$ and $k \leq 5$.
- Randomly sample subgraphs if enumeration is infeasible.

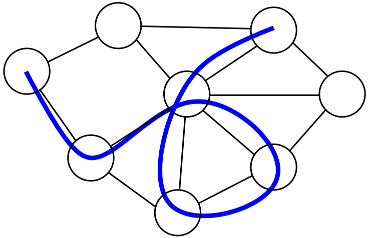
Walks

Definition

- A walk of a graph (V, E) is sequence of $v_1, \ldots, v_n \in V$ such that $(v_i, v_{i+1}) \in E$ for $i = 1, \ldots, n-1$.
- We note $\mathcal{W}_n(G)$ the set of walks with n vertices of the graph G, and $\mathcal{W}(G)$ the set of all walks.



Walks $\neq$ paths



Walk kernel

Definition

- Let $\mathcal{S}_n$ denote the set of all possible label sequences of walks of length n (including vertices and edges labels), and $\mathcal{S} = \cup_{n \geq 1} \mathcal{S}_n$.
- For any graph $\mathcal{X}$ let a weight $\lambda_G(w)$ be associated to each walk $w \in \mathcal{W}(G)$.
- Let the feature vector $\Phi(G) = (\Phi_s(G))_{s \in \mathcal{S}}$ be defined by:

$$\Phi_s(G) = \sum_{w \in \mathcal{W}(G)} \lambda_G(w) \mathbf{1}\,(s \text{ is the label sequence of } w)\ .$$

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- A walk kernel is a graph kernel defined by:

$$K_{walk}(G_1, G_2) = \sum_{s \in \mathcal{S}} \Phi_s(G_1) \Phi_s(G_2) .$$

Walk kernel examples

- The nth-order walk kernel is the walk kernel with $\lambda_G(w) = 1$ if the length of w is n, 0 otherwise. It compares two graphs through their common walks of length n.

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- The random walk kernel is obtained with $\lambda_G(w) = P_G(w)$, where P_G is a Markov random walk on G. In that case we have:

$$K(G_1, G_2) = P(label(W_1) = label(W_2)),$$

where W_1 and W_2 are two independant random walks on G_1 and G_2, respectively (Kashima et al., 2003).

Walk kernel examples

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  where W_1 and W_2 are two independant random walks on G_1 and G_2, respectively (Kashima et al., 2003).
- The geometric walk kernel is obtained (when it converges) with $\lambda_G(w) = \beta^{length(w)}$, for $\beta > 0$. In that case the feature space is of infinite dimension (Gärtner et al., 2003).

Computation of walk kernels

Proposition

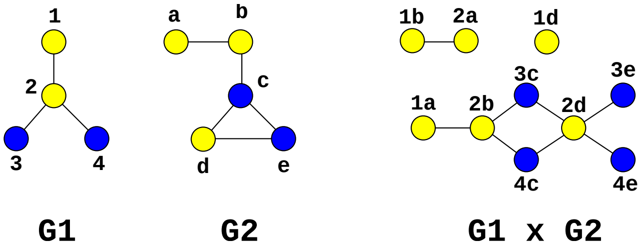
These three kernels (nth-order, random and geometric walk kernels) can be computed efficiently in polynomial time.

Product graph

Definition

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs with labeled vertices. The product graph $G = G_1 \times G_2$ is the graph $G = (V, E)$ with:

1. $V = \{(v_1, v_2) \in V_1 \times V_2 \; : \; v_1 \text{ and } v_2 \text{ have the same label}\}$,
2. $E = \{((v_1, v_2), (v_1', v_2')) \in V \times V \; : \; (v_1, v_1') \in E_1 \text{ and } (v_2, v_2') \in E_2\}$.



Walk kernel and product graph

Lemma

There is a bijection between:

1. The pairs of walks $w_1 \in \mathcal{W}_n(G_1)$ and $w_2 \in \mathcal{W}_n(G_2)$ with the same label sequences,
2. The walks on the product graph $w \in \mathcal{W}_n(G_1 \times G_2)$.

Walk kernel and product graph

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Corollary

$$\begin{aligned}
K_{walk}(G_1, G_2) &= \sum_{s \in \mathcal{S}} \Phi_s(G_1)\Phi_s(G_2) \\
&= \sum_{(w_1,w_2) \in \mathcal{W}(G_1) \times \mathcal{W}(G_1)} \lambda_{G_1}(w_1)\lambda_{G_2}(w_2)\mathbf{1}(l(w_1) = l(w_2)) \\
&= \sum_{w \in \mathcal{W}(G_1 \times G_2)} \lambda_{G_1 \times G_2}(w) \,.
\end{aligned}$$

Computation of the nth-order walk kernel

- For the nth-order walk kernel we have $\lambda_{G_1 \times G_2}(w) = 1$ if the length of w is n, 0 otherwise.
- Therefore:

$$K_{nth-order}(G_1, G_2) = \sum_{w \in \mathcal{W}_n(G_1 \times G_2)} 1 \,.$$

- Let A be the adjacency matrix of $G_1 \times G_2$. Then we get:

$$K_{nth-order}(G_1, G_2) = \sum_{i,j} [A^n]_{i,j} = \mathbf{1}^\top A^n \mathbf{1} \,.$$

- Computation in $O(n|G_1||G_2|d_1 d_2)$, where d_i is the maximum degree of G_i.

Computation of random and geometric walk kernels

- In both cases $\lambda_G(w)$ for a walk $w = v_1 \dots v_n$ can be decomposed as:

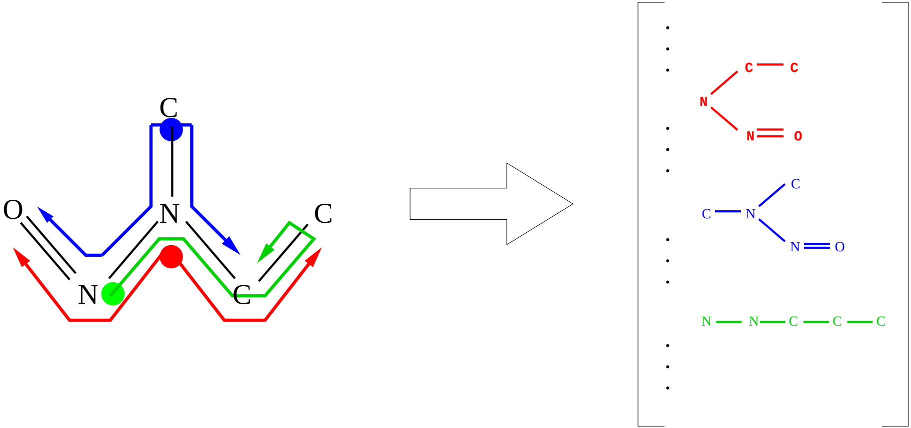
$$\lambda_G(v_1 \dots v_n) = \lambda^i(v_1) \prod_{i=2}^{n} \lambda^t(v_{i-1}, v_i) \,.$$

- Let Λ_i be the vector of $\lambda^i(v)$ and Λ_t be the matrix of $\lambda^t(v, v')$:

$$\begin{aligned} K_{walk}(G_1, G_2) &= \sum_{n=1}^{\infty} \sum_{w \in \mathcal{W}_n(G_1 \times G_2)} \lambda^i(v_1) \prod_{i=2}^{n} \lambda^t(v_{i-1}, v_i) \\ &= \sum_{n=0}^{\infty} \Lambda_i \Lambda_t^n \mathbf{1} \\ &= \Lambda_i \left(I - \Lambda_t\right)^{-1} \mathbf{1} \end{aligned}$$

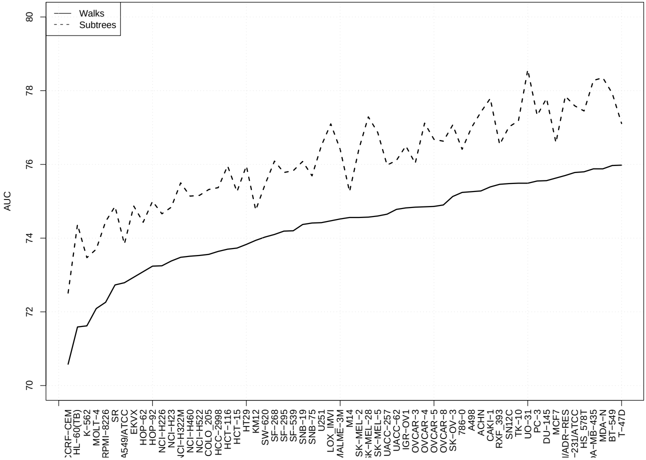
- Computation in $O(|G_1|^3 |G_2|^3)$

Extension: branching walks (Ramon and Gärtner, 2003; Mahé and Vert, 2009)



$$\mathcal{T}(v, n+1) = \sum_{R \subset \mathcal{N}(v)} \prod_{v' \in R} \lambda_t(v, v') \mathcal{T}(v', n),$$

2D Subtree vs walk kernels

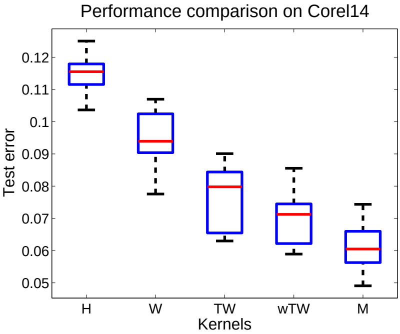


Screening of inhibitors for 60 cancer cell lines.

Image classification (Harchaoui and Bach, 2007)

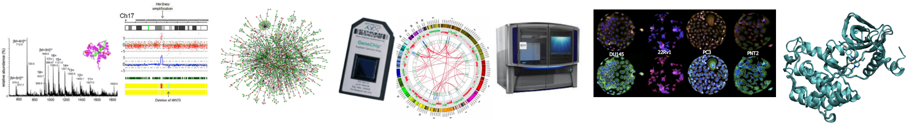
COREL14 dataset

- 1400 natural images in 14 classes
- Compare kernel between histograms (H), walk kernel (W), subtree kernel (TW), weighted subtree kernel (wTW), and a combination (M).



Outline

Motivation



- We have seen how to make learning algorithms given a kernel K on some data space $\mathcal{X}$
- Often we may have several possible kernels:
  - by varying the kernel type or parameters on a given description of the data (eg, linear, polynomial, Gaussian kernels with different bandwidths...)
  - because we have different views of the same data, eg, a protein can be characterized by its sequence, its structure, its mass spectrometry profile...
- How to choose or integrate different kernels in a learning task?

Setting: learning with one kernel

- For any $f : \mathcal{X} \to \mathbb{R}$, let $f^n = (f(x_1), \ldots, f(x_n)) \in \mathbb{R}^n$
- Given a p.d. kernel $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, we learn with K by solving:

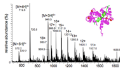
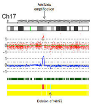
$$\min_{f \in \mathcal{H}} R(f^n) + \lambda \| f \|_{\mathcal{H}}^2 \,, \tag{2}$$

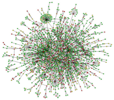
where $\lambda > 0$ and $R : \mathbb{R}^n \to \mathbb{R}$ is an closed[1] and convex empirical risk:

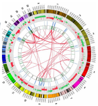
- $R(u) = \frac{1}{n} \sum_{i=1}^n (u_i - y_i)^2$ for kernel ridge regression
- $R(u) = \frac{1}{n} \sum_{i=1}^n \max(1 - y_i u_i, 0)$ for SVM
- $R(u) = \frac{1}{n} \sum_{i=1}^n \log\left(1 + \exp\left(-y_i u_i\right)\right)$ for kernel logistic regression

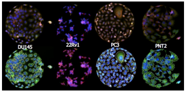
[1] R is closed if, for each $A \in \mathbb{R}$, the sublevel set $\{u \in \mathbb{R}^n : R(u) \leq A\}$ is closed. For example, if R is continuous then it is closed.

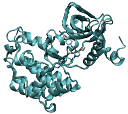
Sum kernel







Definition

Let $K_1, \ldots, K_M$ be M kernels on $\mathcal{X}$. The sum kernel K_S is the kernel on $\mathcal{X}$ defined as

$$\forall x, x' \in \mathcal{X}, \quad K_S(x, x') = \sum_{i=1}^{M} K_i(x, x').$$

Sum kernel and vector concatenation

Theorem

For $i = 1, \ldots, M$, let $\Phi_i : \mathcal{X} \to \mathcal{H}_i$ be a feature map such that

$$K_i(x, x') = \left\langle \Phi_i(x), \Phi_i(x') \right\rangle_{\mathcal{H}_i} .$$

Then $K_S = \sum_{i=1}^{M} K_i$ can be written as:

$$K_S(x, x') = \left\langle \Phi_S(x), \Phi_S(x') \right\rangle_{\mathcal{H}_S} ,$$

where $\Phi_S : \mathcal{X} \to \mathcal{H}_S = \mathcal{H}_1 \oplus \ldots \oplus \mathcal{H}_M$ is the concatenation of the feature maps Φ_i:

$$\Phi_S(x) = (\Phi_1(x), \ldots, \Phi_M(x))^\top .$$

Therefore, summing kernels amounts to concatenating their feature space representations, which is a quite natural way to integrate different features.

Proof

For $\Phi_S(x) = (\Phi_1(x), \ldots, \Phi_M(x))^\top$, we easily compute:

$$\begin{aligned}\left\langle \Phi_S(x), \Phi_S(x') \right\rangle_{\mathcal{H}_s} &= \sum_{i=1}^{M} \left\langle \Phi_i(x), \Phi_i(x') \right\rangle_{\mathcal{H}_i} \\ &= \sum_{i=1}^{M} K_i(x, x') \\ &= K_S(x, x')\,.\end{aligned}$$

Example: data integration with the sum kernel

BIOINFORMATICS

Vol. 20 Suppl. 1 2004, pages i363–i370
DOI: 10.1093/bioinformatics/bth910

Protein network inference from multiple genomic data: a supervised approach

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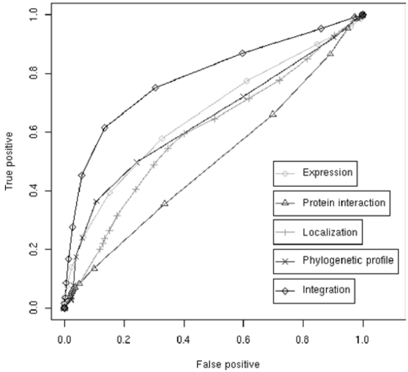
K_{exp} (Expression)
K_{ppi} (Protein interaction)
K_{loc} (Localization)
K_{phy} (Phylogenetic profile)
$K_{\text{exp}} + K_{\text{ppi}} + K_{\text{loc}} + K_{\text{phy}}$ (Integration)



The sum kernel: functional point of view

Theorem

The solution $f^* \in \mathcal{H}_{K_S}$ when we learn with $K_S = \sum_{i=1}^M K_i$ is equal to:

$$f^* = \sum_{i=1}^M f_i^* \,,$$

where $(f_1^*, \ldots, f_M^*) \in \mathcal{H}_{K_1} \times \ldots \times \mathcal{H}_{K_M}$ is the solution of:

$$\min_{f_1,\ldots,f_M} R\left(\sum_{i=1}^M f_i^n\right) + \lambda \sum_{i=1}^M \| f_i \|^2_{\mathcal{H}_{K_i}} \,.$$

Generalization: The weighted sum kernel

Theorem

The solution f^* when we learn with $K_\eta = \sum_{i=1}^M \eta_i K_i$, with $\eta_1, \ldots, \eta_M \geq 0$, is equal to:

$$f^* = \sum_{i=1}^M f_i^* \,,$$

where $(f_1^*, \ldots, f_M^*) \in \mathcal{H}_{K_1} \times \ldots \times \mathcal{H}_{K_M}$ is the solution of:

$$\min_{f_1, \ldots, f_M} R\left(\sum_{i=1}^M f_i^n\right) + \lambda \sum_{i=1}^M \frac{\| f_i \|_{\mathcal{H}_{K_i}}^2}{\eta_i} \,.$$

Proof (1/4)

$$\min_{f_1,\ldots,f_M} R\left(\sum_{i=1}^{M} f_i^n\right) + \lambda \sum_{i=1}^{M} \frac{\| f_i \|^2_{\mathcal{H}_{K_i}}}{\eta_i} .$$

- R being convex, the problem is strictly convex and has a unique solution $(f_1^*, \ldots, f_M^*) \in \mathcal{H}_{K_1} \times \ldots \times \mathcal{H}_{K_M}$.
- By the representer theorem, there exists $\alpha_1^*, \ldots, \alpha_M^* \in \mathbb{R}^n$ such that

$$f_i^*(x) = \sum_{j=1}^{n} \alpha_{ij}^* K_i(x_j, x) .$$

- $(\alpha_1^*, \ldots, \alpha_M^*)$ is the solution of

$$\min_{\alpha_1,\ldots,\alpha_M \in \mathbb{R}^n} R\left(\sum_{i=1}^{M} K_i \alpha_i\right) + \lambda \sum_{i=1}^{M} \frac{\alpha_i^\top K_i \alpha_i}{\eta_i} .$$

Proof (2/4)

- This is equivalent to

$$\min_{u,\alpha_1,\dots,\alpha_M\in\mathbb{R}^n} R(u) + \lambda\sum_{i=1}^{M}\frac{\alpha_i^\top K_i\alpha_i}{\eta_i} \quad \text{s.t.} \quad u = \sum_{i=1}^{M} K_i\alpha_i\,.$$

- This is equivalent to the saddle point problem:

$$\min_{u,\alpha_1,\dots,\alpha_M\in\mathbb{R}^n}\ \max_{\gamma\in\mathbb{R}^n} R(u) + \lambda\sum_{i=1}^{M}\frac{\alpha_i^\top K_i\alpha_i}{\eta_i} + 2\lambda\gamma^\top\Big(u - \sum_{i=1}^{M} K_i\alpha_i\Big)\,.$$

- By Slater's condition, strong duality holds, meaning we can invert min and max:

$$\max_{\gamma\in\mathbb{R}^n}\ \min_{u,\alpha_1,\dots,\alpha_M\in\mathbb{R}^n} R(u) + \lambda\sum_{i=1}^{M}\frac{\alpha_i^\top K_i\alpha_i}{\eta_i} + 2\lambda\gamma^\top\Big(u - \sum_{i=1}^{M} K_i\alpha_i\Big)\,.$$

Proof (3/4)

- Minimization in u:

$$\min_u R(u) + 2\lambda\gamma^\top u = -\max_u \left\{-2\lambda\gamma^\top u - R(u)\right\} = -R^*(-2\lambda\gamma)\,,$$

  where R^* is the Fenchel dual of R:

$$\forall v \in \mathbb{R}^n \quad R^*(v) = \sup_{u\in\mathbb{R}^n} u^\top v - R(u)\,.$$

- Minimization in α_i for $i = 1, \ldots, M$:

$$\min_{\alpha_i} \left\{\lambda \frac{\alpha_i^\top K_i \alpha_i}{\eta_i} - 2\lambda\gamma^\top K_i\alpha_i\right\} = -\lambda\eta_i\gamma^\top K_i\gamma\,,$$

  where the minimum in α_i is reached for $\alpha_i^* = \eta_i\gamma$.

Proof (4/4)

- The dual problem is therefore

$$\max_{\gamma \in \mathbb{R}^n} \left\{ -R^*(-2\lambda\gamma) - \lambda\gamma^\top \left(\sum_{i=1}^{M} \eta_i K_i \right) \gamma \right\} .$$

- Note that if learn from a single kernel K_η, we get the same dual problem

$$\max_{\gamma \in \mathbb{R}^n} \left\{ -R^*(-2\lambda\gamma) - \lambda\gamma^\top K_\eta \gamma \right\} .$$

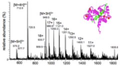
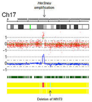
- If γ^* is a solution of the dual problem, then $\alpha_i^* = \eta_i \gamma^*$ leading to:

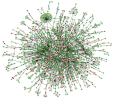
$$\forall x \in \mathcal{X} , \quad f_i^* (x) = \sum_{j=1}^{n} \alpha_{ij}^* K_i (x_j, x) = \sum_{j=1}^{n} \eta_i \gamma_j^* K_i (x_j, x)$$

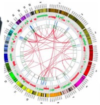
- Therefore, $f^* = \sum_{i=1}^{M} f_i^*$ satisfies

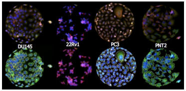
$$f^* (x) = \sum_{i=1}^{M} \sum_{j=1}^{n} \eta_i \gamma_j^* K_i (x_j, x) = \sum_{j=1}^{n} \gamma_j^* K_\eta (x_j, x) . \quad \square$$

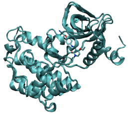
Learning the kernel









Motivation

- If we know how to weight each kernel, then we can learn with the weighted kernel

$$K_\eta = \sum_{i=1}^{M} \eta_i K_i$$

- However, usually we don't know...
- Perhaps we can optimize the weights η_i during learning?

An objective function for K

Theorem

For any p.d. kernel K on $\mathcal{X}$, let

$$J(K) = \min_{f \in \mathcal{H}} \left\{ R(f^n) + \lambda \| f \|_{\mathcal{H}}^2 \right\} .$$

The function $K \mapsto J(K)$ is convex.

This suggests a principled way to "learn" a kernel: define a convex set of candidate kernels, and minimize $J(K)$ by convex optimization.

Proof

- We have shown by strong duality that

$$J(K) = \max_{\gamma \in \mathbb{R}^n} \left\{ -R^*(-2\lambda\gamma) - \lambda\gamma^\top K\gamma \right\} .$$

- For each γ fixed, this is an affine function of K, hence convex
- A supremum of convex functions is convex. $\square$

MKL (Lanckriet et al., 2004)

- We consider the set of convex combinations

$$K_\eta = \sum_{i=1}^{M} \eta_i K_i \quad \text{with} \quad \eta \in \Sigma_M = \left\{ \eta_i \geq 0 \, , \, \sum_{i=1}^{M} \eta_i = 1 \right\}$$

- We optimize both η and f^* by solving:

$$\min_{\eta \in \Sigma_M} J\left(K_\eta\right) = \min_{\eta \in \Sigma_M} \min_{f \in \mathcal{H}_{K_\eta}} \left\{ R(f^n) + \lambda \| f \|^2_{\mathcal{H}_{K_\eta}} \right\}$$

- The problem is jointly convex in (η, α) and can be solved efficiently.
- The output is both a set of weights η, and a predictor corresponding to the kernel method trained with kernel K_η.
- This method is usually called Multiple Kernel Learning (MKL).

Example: protein annotation

BIOINFORMATICS

Vol. 20 no. 16 2004, pages 2626–2635
doi:10.1093/bioinformatics/bth294

A statistical framework for genomic data fusion

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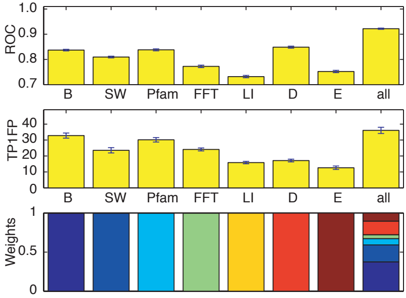
Kernel	Data	Similarity measure
K_{SW}	protein sequences	Smith-Waterman
K_{B}	protein sequences	BLAST
K_{Pfam}	protein sequences	Pfam HMM
K_{FFT}	hydropathy profile	FFT
K_{LI}	protein interactions	linear kernel
K_{D}	protein interactions	diffusion kernel
K_{E}	gene expression	radial basis kernel
K_{RND}	random numbers	linear kernel

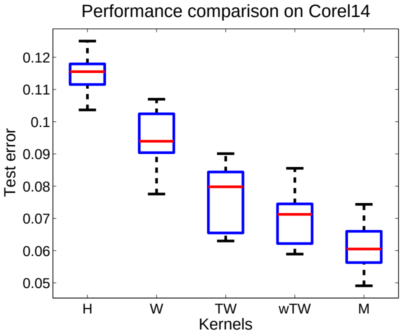


(B) Membrane proteins

Example: Image classification (Harchaoui and Bach, 2007)

COREL14 dataset

- 1400 natural images in 14 classes
- Compare kernel between histograms (H), walk kernel (W), subtree kernel (TW), weighted subtree kernel (wTW), and a combination by MKL (M).



MKL revisited (Bach et al., 2004)

$$K_\eta = \sum_{i=1}^{M} \eta_i K_i \quad \text{with} \quad \eta \in \Sigma_M = \left\{ \eta_i \geq 0 \, , \, \sum_{i=1}^{M} \eta_i = 1 \right\}$$

Theorem

The solution f^* of

$$\min_{\eta \in \Sigma_M} \min_{f \in \mathcal{H}_{K_\eta}} \left\{ R(f^n) + \lambda \| \, f \, \|^2_{\mathcal{H}_{K_\eta}} \right\}$$

is $f^* = \sum_{i=1}^{M} f_i^*$, where $(f_1^*, \ldots, f_M^*) \in \mathcal{H}_{K_1} \times \ldots \times \mathcal{H}_{K_M}$ is the solution of:

$$\min_{f_1, \ldots, f_M} \left\{ R\left(\sum_{i=1}^{M} f_i^n \right) + \lambda \left(\sum_{i=1}^{M} \| \, f_i \, \|_{\mathcal{H}_{K_i}} \right)^2 \right\} .$$

Proof (1/2)

$$
\begin{aligned}
\min_{\eta \in \Sigma_M} \min_{f \in \mathcal{H}_{K_\eta}} & \left\{ R(f^n) + \lambda \| f \|^2_{\mathcal{H}_{K_\eta}} \right\} \\
&= \min_{\eta \in \Sigma_M} \min_{f_1, \ldots, f_M} \left\{ R\left(\sum_{i=1}^M f_i^n \right) + \lambda \sum_{i=1}^M \frac{\| f_i \|^2_{\mathcal{H}_{K_i}}}{\eta_i} \right\} \\
&= \min_{f_1, \ldots, f_M} \left\{ R\left(\sum_{i=1}^M f_i^n \right) + \lambda \min_{\eta \in \Sigma_M} \left\{ \sum_{i=1}^M \frac{\| f_i \|^2_{\mathcal{H}_{K_i}}}{\eta_i} \right\} \right\} \\
&= \min_{f_1, \ldots, f_M} \left\{ R\left(\sum_{i=1}^M f_i^n \right) + \lambda \left(\sum_{i=1}^M \| f_i \|_{\mathcal{H}_{K_i}} \right)^2 \right\} ,
\end{aligned}
$$

Proof (2/2)

where the last equality results from:

$$\forall a \in \mathbb{R}_+^M\,, \quad \left(\sum_{i=1}^M a_i\right)^2 = \inf_{\eta \in \Sigma_M} \sum_{i=1}^M \frac{a_i^2}{\eta_i}\,,$$

which is a direct consequence of the Cauchy-Schwarz inequality:

$$\sum_{i=1}^M a_i = \sum_{i=1}^M \frac{a_i}{\sqrt{\eta_i}} \times \sqrt{\eta_i} \leq \left(\sum_{i=1}^M \frac{a_i^2}{\eta_i}\right)^{\frac{1}{2}} \left(\sum_{i=1}^M \eta_i\right)^{\frac{1}{2}}\,.$$

Algorithm: simpleMKL (Rakotomamonjy et al., 2008)

- We want to minimize in $\eta \in \Sigma_M$:

$$\min_{\eta \in \Sigma_M} J(K_\eta) = \min_{\eta \in \Sigma_M} \max_{\gamma \in \mathbb{R}^n} \left\{ -R^*(-2\lambda\gamma) - \lambda\gamma^\top K_\eta \gamma \right\} .$$

- For a fixed $\eta \in \Sigma_M$, we can compute $f(\eta) = J(K_\eta)$ by using a standard solver for a single kernel to find γ^*:

$$J(K_\eta) = -R^*(-2\lambda\gamma^*) - \lambda\gamma^{*\top} K_\eta \gamma^* .$$

- From γ^* we can also compute the gradient of $J(K_\eta)$ with respect to η:

$$\frac{\partial J(K_\eta)}{\partial \eta_i} = -\lambda\gamma^{*\top} K_i \gamma^* .$$

- $J(K_\eta)$ can then be minimized on Σ_M by a projected gradient or reduced gradient algorithm.

Sum kernel vs MKL

- Learning with the sum kernel (uniform combination) solves

$$\min_{f_1,\ldots,f_M} \left\{ R\left(\sum_{i=1}^{M} f_i^n\right) + \lambda \sum_{i=1}^{M} \| f_i \|_{\mathcal{H}_{K_i}}^2 \right\} .$$

- Learning with MKL (best convex combination) solves

$$\min_{f_1,\ldots,f_M} \left\{ R\left(\sum_{i=1}^{M} f_i^n\right) + \lambda \left(\sum_{i=1}^{M} \| f_i \|_{\mathcal{H}_{K_i}}\right)^2 \right\} .$$

- Although MKL can be thought of as optimizing a convex combination of kernels, it is more correct to think of it as a penalized risk minimization estimator with the group lasso penalty:

$$\Omega(f) = \min_{f_1+\ldots+f_M=f} \sum_{i=1}^{M} \| f_i \|_{\mathcal{H}_{K_i}} .$$

Example: ridge vs LASSO regression

- Take $\mathcal{X} = \mathbb{R}^d$, and for $x = (x_1, \ldots, x_d)^\top$ consider the rank-1 kernels:

$$\forall i = 1, \ldots, d\,, \quad K_i\left(x, x'\right) = x_i x_i'\,.$$

- A function $f_i \in \mathcal{H}_{K_i}$ has the form $f_i(x) = \beta_i x_i$, with $\| f_i \|_{\mathcal{H}_{K_i}} = |\, \beta_i \,|$
- The sum kernel is $K_S(x, x') = \sum_{i=1}^d x_i x_i' = x^\top x$, a function $\mathcal{H}_{K_S}$ is of the form $f(x) = \boldsymbol{\beta}^\top x$, with norm $\| f \|_{\mathcal{H}_{K_S}} = \| \boldsymbol{\beta} \|_{\mathbb{R}^d}$.
- Learning with the sum kernel solves a ridge regression problem:

$$\min_{\boldsymbol{\beta} \in \mathbb{R}^d} \left\{ R(X\boldsymbol{\beta}) + \lambda \sum_{i=1}^d \beta_i^2 \right\}\,.$$

- Learning with MKL solves a LASSO regression problem:

$$\min_{\boldsymbol{\beta} \in \mathbb{R}^d} \left\{ R(X\boldsymbol{\beta}) + \lambda \left(\sum_{i=1}^d |\, \beta_i \,| \right)^2 \right\}\,.$$

Extensions (Micchelli et al., 2005)

$$\text{For } r > 0\,, \quad K_\eta = \sum_{i=1}^{M} \eta_i K_i \quad \text{with} \quad \eta \in \Sigma_M^r = \left\{ \eta_i \geq 0\,,\, \sum_{i=1}^{M} \eta_i^r = 1 \right\}$$

Theorem

The solution f^* of

$$\min_{\eta \in \Sigma_M^r} \min_{f \in \mathcal{H}_{K_\eta}} \left\{ R(f^n) + \lambda \| f \|^2_{\mathcal{H}_{K_\eta}} \right\}$$

is $f^* = \sum_{i=1}^{M} f_i^*$, where $(f_1^*, \ldots, f_M^*) \in \mathcal{H}_{K_1} \times \ldots \times \mathcal{H}_{K_M}$ is the solution of:

$$\min_{f_1, \ldots, f_M} \left\{ R\left(\sum_{i=1}^{M} f_i^n \right) + \lambda \left(\sum_{i=1}^{M} \| f_i \|^{\frac{2r}{r+1}}_{\mathcal{H}_{K_i}} \right)^{\frac{r+1}{r}} \right\}.$$

Outline

In one slide...

- Learning in high dimension requires regularization, e.g., by ℓ_2 penalty for linear methods
- Kernels allow to transform any ℓ_2-regularized linear models into a nonlinear model, thanks to the kernel trick
- There exists many kernels, which correspond to different feature spaces (of finite or infinite dimensions)
- We can combine and learn kernels, e.g., for integration of heterogeneous data
- Hot research topics
    - Large-scale ML with kernels
    - Deep kernel methods

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MURAKOZE

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